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THE UNIVERSITY OF ALBERTA

# MODELLING OF AMINE UNITS AND MULTICOLUMN SYSTEMS

by

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A THESIS
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FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled "MODELLING OF AMINE UNITS AND MULTICOLUMN SYSTEMS", submitted by Denis Wakefield Browne, in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

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# ABSTRACT

The calculational method for multistage, multicomponent separation processes developed by Ishii has been utilized to build a computational model for amine contactors and regenerators. Use of the model is illustrated with test problems typical of columns operating in natural gas processing plants. Two correlations of experimental solubility data are used in the problems and the results are shown to be sensitive to the correlation employed. Some consideration is also given to the use and estimation of stage efficiencies. The incorporation of efficiencies is shown to be important in an accurate design; however the accuracy of calculated values is limited by a paucity of reliable rate data.

In addition, Ishii's method has been extended to produce an algorithm for the solution of multicolumn configurations. The algorithm utilizes the basic block tridiagonal matrix form of the linearized steady state equations and the sparseness of many of the matrices to produce a quick and efficient solution procedure. The algorithm has shown reliability in converging for the three systems tried, namely a thermally coupled distillation system, an extractive distillation system and an amine treating system. However, some problems are encountered with certain column specifications.

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# TABLE OF CONTENTS

CHAPTER PAGE

1. INTRODUCTION 1

2. LITERATURE REVIEW 5

   2.1 Design Methods for Alkanolamine Units 5

   2.2 Correlation of Equilibrium Solubility Data For $H_2S$ and $CO_2$ in Alkanolamine Solutions 7

   2.3 Enthalpy Data for Acid Gas-Amine Systems 12

   2.4 Numerical Solution of Stagewise Processes for Multicomponent Mixtures 13

      2.4.1 Algorithms for Equilibrium Stage Calculations 13

      2.4.2 Stage Efficiencies 15

   2.5 Stage Efficiencies for Amine Units 18

   2.6 Multicolumn Calculations 21

3. MODELLING AMINE CONTACTORS AND REGENERATORS 25

   3.1 Stage Model 25

      3.1.1 Solution Procedure 28

      3.1.2 Initial Assumptions 30

   3.2 Determination of Equilibrium K-ratios 34

   3.3 Determination of Enthalpies 36

   3.4 Development of Partial Derivatives 37

## TABLE OF CONTENTS

CHAPTER PAGE

4. APPLICATION OF THE MODEL TO THE DESIGN OF AMINE UNITS 43

4.1 Test Problems 43

4.2 Discussion of Test Problems 51

4.3 Dependence of Sweet Gas $H_2S$ Composition on Lean Amine Residuals 55

4.4 Prediction of Stage Efficiencies 58

4.4.1 $CO_2$ Stage Efficiency 60

4.4.2 $H_2S$ Stage Efficiency 62

4.4.3 Example Problem No. 5 63

5. A GENERAL ALGORITHM FOR SOLVING MULTICOLUMN SYSTEMS 66

5.1 Model Equations 66

5.2 Linearized Equations 69

5.3 Matrix Forms 74

5.4 Effect of Problem Specifications on Matrix Elements 85

5.5 Solution Procedure 88

6. USE OF THE MULTICOLUMN ALGORITHM 94

6.1 Example Problems 94

6.2 Results and Discussion 104

6.2.1 Evaluation of the Algorithm 105

6.2.2 Example Problem 1 108

## TABLE OF CONTENTS

CHAPTER PAGE

6.2.3 Example Problem 2 109

6.2.4 Example Problem 3 112

6.3 Application to the Design of Amine Treating Systems 114

6.3.1 The Split Flow System Option 114

6.3.2 Choice of a Stripping Steam Rate to Achieve a Given Lean Amine Residual 116

7. CONCLUSIONS 121

NOMENCLATURE 124

REFERENCES 130

APPENDIX

1. Enthalpies of Solution of $CO_2$ and $H_2S$ in MEA and DEA Solutions 133

2. Constants in Correlations for Ideal Gas Enthalpy and Latent Heat of Vapourization 136

3. Intermediate Partial Derivatives Required in the Derivation of $\partial K/\partial x$ for $H_2S$ and $CO_2$ 138

4. Computer Printouts for Amine Contactor and Regenerator Problems 146

# TABLE OF CONTENTS

APPENDIX PAGE

4.1 Test Problem 1 - Nasir Correlation 147
4.2 Test Problem 2 - Nasir Correlation 152
4.3 Test Problem 3 - Nasir Correlation 156
4.4 Test Problem 4 - Nasir Correlation 161
4.5 Test Problem 1 - Amoco Correlation 167
4.6 Test Problem 2 - Amoco Correlation 172
4.7 Test Problem 3 - Amoco Correlation 176
4.8 Test Problem 4 - Amoco Correlation 181
4.9 Test Problem 5 - Nasir Correlation 186

5. Equilibrium and Enthalpy Data for Extractive Distillation Problem 192

6. Computer Printouts for Problems Using Linked Column Algorithm 197
6.1 Thermally Coupled Distillation System 198
6.2 Extractive Distillation System 209
6.3 Amine Treating System 225

# LIST OF TABLES

| TABLE | | PAGE |
|---|---|---|
| 1 | Henry's Law Coefficient (atm/mole fraction) For $CO_2$ and $H_2S$ in Water | 12 |
| 2 | Number of Iterations and CPU Times Required for Test Problems for Two Data Correlations | 51 |
| 3 | Comparison of the Values of Important Design Variables | 52 |
| 4 | Murphree Efficiencies as Calculated From Vapourization Efficiencies | 65 |
| 5 | Contribution of Interlinked Streams to Material and Energy Balance Equations | 69 |
| 6 | Terms in Linearized Equations Arising from Interconnected Streams | 73 |
| 7 | Non-zero Off-tridiagonal Elements in Each Coefficient Matrix | 79 |
| 8 | Convergence Characteristics and CPU Times for Linked Column Example Problems | 104 |
| 9 | Comparison of Runs for Thermally Coupled Distillation Problem | 109 |
| 10 | Comparison of Results Given by Split Flow and Conventional Configurations | 116 |
| 11 | $H_2S$ and $CO_2$ Lean Amine Residuals for Different Reboiler Stream Rates and Acid Gas Ratios in the Feed | 117 |

## LIST OF FIGURES

| FIGURE | | PAGE |
|---|---|---|
| 1 | Amine Sweetening System | 2 |
| 2 | Generalized Stage Model | 26 |
| 3 | Composition of $H_2S$ in Sweet Gas Versus $H_2S$ Lean Amine Residual | 56 |
| 4 | General Stage in a Multicolumn System | 67 |
| 5 | Example System of Columns | 76 |
| 6 | General Matrix Form | 77 |
| 7 | Thermally Coupled Distillation System | 95 |
| 8 | Extractive Distillation System | 99 |
| 9 | Acid Gas Lean Amine Residuals Versus Acid Gas Feed Ratio at Different Steam Rates | 118 |

# 1. INTRODUCTION

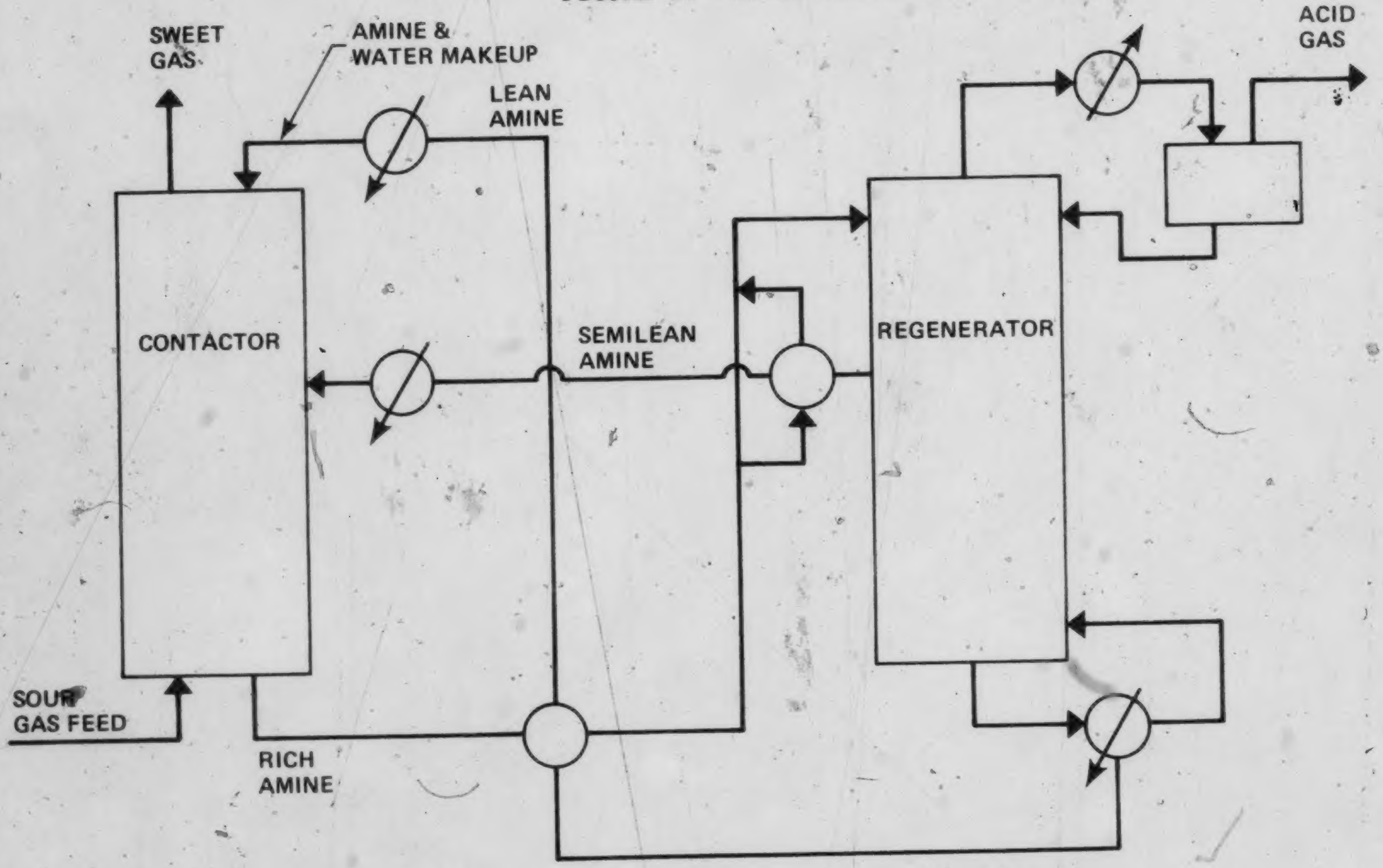
In the gas processing industry the removal of acid gases $H_2S$ and $CO_2$ from gas streams is of prime importance. Alkanolamines are widely used to effect this removal, particularly from streams such as the hydrocarbon streams encountered in natural gas processing, in petroleum refining and in the upgrading of bitumen obtained from oil sands. Also, in the production of ammonia alkanolamines are used to remove $CO_2$ from the synthesis gas stream.

The normal flowsheet configuration of a gas sweetening system using alkanolamines is shown as Figure 1. Sour gas feed is contacted with a lean amine stream containing small quantities of $H_2S$ and $CO_2$. The resulting sweet gas stream contains $H_2S$ and $CO_2$ to the extent of ppm; with a typical specification on $H_2S$ being less than 0.25 grain per 100 SCF (approximately 4 ppm). The rich amine is fed to a regenerator in which essentially all the acid gas components are removed as overhead product, producing as bottoms product the lean amine which is recycled to the top contactor stage.

A small makeup of amine and water is needed to counter vapourization losses. The semilean amine stream is an optional innovation that may reduce operating costs.

In the design of an amine system the important

FIGURE 1: AMINE SWEETENING SYSTEM


SWEET GAS
AMINE & WATER MAKEUP
LEAN AMINE
ACID GAS
CONTACTOR
SEMILEAN AMINE
REGENERATOR
SOUR GAS FEED
RICH AMINE

information required includes:

(i) the number of stages in each column
(ii) type of amine and solution concentration
(iii) the amine circulation rate
(iv) steam requirements in the regenerator.

The absorption of $H_2S$ and $CO_2$ in alkanolamine solutions is complex in that it involves simultaneous absorption and chemical reaction, and rate and equilibrium data are scarce for such systems. As a result amine systems are most often designed on the basis of "rules-of-thumb" derived from experience. Typical examples are the use of approximately 20 stages in the towers, regenerator steam loads of between 1.0 and 1.2 lb. of steam per gallon of circulating amine, circulation rates based on a pickup of 2.5 SCF acid gas per gallon of amine, and the choice of MEA solution concentrations of 15 weight percent. The use of these "rules-of-thumb" no doubt fails to produce an optimum design in many cases. Thus there is a need for a better design procedure.

This study was undertaken to develop a computer oriented design procedure which would make use of recent advances in two areas namely:

(i) techniques for making stagewise calculations for multicomponent mixtures, based on the equilibrium stage concept.

(ii) developments [illegible] the preparation of thermodynamically based correlations of equilibrium solubility data for $H_2S$ and $CO_2$ in alkanolamine solutions.

Considering that the amines have a different selectivity for $H_2S$ than for $CO_2$, the stage efficiency becomes an important consideration in an accurate simulation or design. Thus some attention is given to the use and estimation of stage efficiencies.

An additional aim of the study is to extend the method described by Ishii and Otto[18] for multistage, multicomponent equilibrium stage calculations to multicolumn systems. Part of the motivation for this is that amine systems involve recycle streams, in particular the lean amine and the semilean amine. The latter is an option in which a partially regenerated amine stream is recycled from the regenerator to the middle section of the contactor. There is some dispute over the usefulness of this configuration and an adequate model of the system will permit an accurate evaluation to be made.

# 2. LITERATURE REVIEW

## 2.1 Design Methods for Alkanolamine Units

Most current design techniques for alkanolamine units rely heavily on empirical "rules-of-thumb". In particular, it is common practice to use 20 stages for the contactor, and a similar standard number for the regenerator[24]. The circulation rate is estimated from either an assumed acid gas pickup per gallon of amine solution[30], or from a limit on the acid gas loading in the rich amine, and steam requirements for the regenerator are assigned as a standard quantity of steam per gallon of circulating amine[30].

The above practices are known to overdesign units and so certain refinements to design procedures have been proposed, primarily by Kohl and Riesenfeld[24] and Maddox[30]. The circulation rate has a considerable effect on capital and operating costs, and both authors attempt to calculate this rate more accurately. The basis is to assume a percentage approach to equilibrium on the bottom stage, with values used lying between 65% and 75%[30]. Equivalently, a minimum circulation rate can be estimated on the assumption of equilibrium existing on the bottom stage, and the actual rate obtained by multiplying this minimum rate by an empirically determined factor[24,29].

Another major design variable is the reboiler heat requirement. Fitzgerald and Richardson[9] used data from a number of operating MEA plants to prepare a widely used empirical correlation which relates the residual $H_2S$ in the lean amine solution, the ratio of $H_2S:CO_2$ in the feed and the steam rate, expressed in lb/gal. A similar chart exists for the $CO_2$ lean amine residual.

The so-called "split-stream" process, attributed to Shoeld[40], has achieved some measure of attention. The process reduces the energy requirements in the reboiler[24], and is claimed to have particular advantage for gas streams containing more than 30 percent acid gas[30]. However, capital investment in a "split-stream" plant is higher than in a conventional plant, because of added complexity in mechanical design, and added pumping and heat exchange costs.

Selection of the type of amine is dictated somewhat by the presence or absence of COS and $CS_2$, which undergo irreversible reactions with MEA[24]. The concentration of the solution is also restricted by corrosion considerations[30], and this is one major reason for using 15 weight percent MEA.

Most authors regard the complexity of the reactions inside the contactor as sufficient justification for using a standard number of stages. However, Kohl and Riesenfeld[24] suggest the number of stages can be estimated on the basis of an empirical correlation for the mass transfer coefficient and stage efficiency for $CO_2$. Average values are used for all stages and the presence of $H_2S$ ignored.

One detailed stagewise calculation of an acid gas absorber has been published, by Rowland and Grens[39]. Solutions with only one acid gas component are used and a number of simplifying assumptions are made. For example the individual phase mass transfer coefficients are assumed constant on all stages. No detail is given of the method of obtaining equilibrium and enthalpy data. The authors compared stage-to-stage and Thiele-Geddes type calculations and concluded that a stage-to-stage technique is the more effective technique for real stage acid gas absorbers.

## 2.2 Correlation of Equilibrium Solubility Data For $H_2S$ and $CO_2$ in Alkanolamine Solutions.

Equilibrium solubility data may be correlated by curve fitting the available data, or alternatively a predictive model can be established based on a suitable set of chemical reactions. For the case of $H_2S$ and $CO_2$ in an aqueous amine solution, the following set of reactions can be written[35]:

$$RNH_2 + H_2O \rightleftharpoons RNH_3^+ + OH^- \qquad (2\text{-}1\text{-}a)$$

$$H_2O \rightleftharpoons H^+ + OH^- \qquad (2\text{-}1\text{-}b)$$

$$H_2S \rightleftharpoons H^+ + HS^- \qquad (2\text{-}1\text{-}c)$$

$$HS^- \rightleftharpoons H^+ + S^{2-} \qquad (2\text{-}1\text{-}d)$$

$$2RNH_2 + CO_2 \rightleftharpoons RNH_3^+ + RNHCOO^- \qquad (2\text{-}1\text{-}e)$$

$$CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^- \qquad (2\text{-}1\text{-}f)$$

$$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-} \qquad (2\text{-}1\text{-}g)$$

$$H_2S(g) \rightleftharpoons H_2S(\ell) \qquad (2\text{-}1\text{-}h)$$

$$CO_2(g) \rightleftharpoons CO_2(\ell) \qquad (2\text{-}1\text{-}i)$$

Where R denotes the group $-CH_2-CH_2-OH$. If R-H in the above equations is replaced by R-R, then the equations represent the chemical reactions in the $H_2S$-$CO_2$-DEA-water system.

In addition, three mass balances and an electroneutrality balance can be written, namely:

$$[RNH_2] + [RNHCOO^-] + [RNH_3^+] = \underset{\text{(amine molality)}}{m} \qquad (2\text{-}2\text{-}a)$$

$$[HS^-] + [H_2S] + [S^{2-}] = \underset{\text{(}H_2S\text{ molality)}}{mX_{H_2S}} \qquad (2\text{-}2\text{-}b)$$

$$[HCO_3^-]+[CO_2]+[CO_3^{2-}]+[RNHCOO^-] = mX_{CO_2}$$

(CO$_2$ molality)

(2-2-c)

$$[RNH_3^+]+[H^+]-([HCO_3^-]+[RNHCOO^-]+2[CO_3^{2-}]+[OH^-]+[HS^-]+2[S^{2-}]) = 0 \qquad (2\text{-}2\text{-}d)$$

Both Klyamer et al.[22] and Nasir[35] have developed models based on this set of equations. In the former model, non-idealities in the liquid phase are accounted for by using activity coefficients. Nasir[35] extended this refinement to include:

(a) vapour phase fugacities to account for deviations from ideal conditions at low temperatures and high pressures.

(b) an additional dependence of the activity coefficient on temperature and molality of alkanolamine, rather than just on ionic strength.

(c) empirical corrections to the partial pressures of $H_2S$ and $CO_2$ in the region of very low acid gas loadings, where the predicted values deviate markedly from the experimental values.

For both models the following set of thermodynamic equilibrium constant expressions for equations (2-1-a) to (2-1-i) may be written:

$$K_i = \frac{\gamma^2}{a\alpha^2} \frac{[RNH_3^+][OH^-]}{[RNH_2]} \qquad (2\text{-}3\text{-}a)$$

$$K_w = \frac{\gamma^2}{\alpha} [H^+][OH^-] \qquad (2\text{-}3\text{-}b)$$

$$K_{1c} = \gamma^2 \frac{[H^+][HS^-]}{[H_2S]} \qquad (2\text{-}3\text{-}c)$$

$$K_{2c} = \gamma \frac{[H^+][S^{2-}]}{[HS^-]} \qquad (2\text{-}3\text{-}d)$$

$$K_m = \frac{\gamma^2}{a^2\alpha^2} \frac{[RNH_3^+][RNHCOO^-]}{[RNH_2]^2 P_{CO_2}} \qquad (2\text{-}3\text{-}e)$$

$$K_{1y} = \frac{\gamma^2}{\alpha} \frac{[H^+][HCO_3^-]}{[CO_2]} \qquad (2\text{-}3\text{-}f)$$

$$K_{2y} = \gamma \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} \qquad (2\text{-}3\text{-}g)$$

$$H_{CO_2} = [CO_2]/P_{CO_2} \qquad (2\text{-}3\text{-}h)$$

$$H_{H_2S} = [H_2S]/P_{H_2S} \qquad (2\text{-}3\text{-}i)$$

where: $\gamma$ is the average coefficient for the ion activity (assumed equal for all ions in solution)

$\alpha$ is the water activity (assumed equal to its molarity)

a is the ratio between the un-ionized ethanolamine activity and the activity of water.

$P_{CO_2}$, $P_{H_2S}$ are the partial pressures of $CO_2$ and $H_2S$ in mm Hg.

Equations (2-3-a) and (2-3-i) may be simplified into implicit expressions in $P_{CO_2}$ and $P_{H_2S}$ which can be solved numerically. The expressions[35] are:

$$P_{H_2S} = \frac{K_W}{K_i K_{1c} H_{H_2S}} \cdot \frac{\gamma^2}{a\alpha} \cdot \frac{A(A+B)}{(m-z-A-B)} \qquad (2\text{-}4)$$

$$P_{CO_2} = \frac{1}{K_m} \cdot \frac{\gamma^2}{a^2\alpha^2} \cdot \frac{z(A+B)}{(m-z-A-B)^2} \qquad (2\text{-}5)$$

where A and B depend on $P_{H_2S}$ and $P_{CO_2}$ respectively.

AMOCO[25] derived a solubility model based on a different, but chemically equivalent[35], set of reactions to equations (2-1-a) to (2-1-i). Details of the model cannot be disclosed here.

A different approach to the above was taken by Kent and Eisenberg[21], who combined all the non-idealities into two parameters. These parameters were curve fitted using available equilibrium data. The model works best for pure component systems, but shows marked deviations in mixtures[35].

In the condenser of the regenerator, the liquid phase is essentially all water. Thus a simple Henry's Law model of $H_2S$ and $CO_2$ in water may be used. The relevant data taken from Perry[6] are given in Table 1.

TABLE 1: HENRY'S LAW COEFFICIENT
(atm/mole fraction)
FOR $CO_2$ AND $H_2S$ IN WATER

| t,°C | 30 | 35 | 40 | 45 | 50 | 60 |
|---|---|---|---|---|---|---|
| $H_{CO_2} \times 10^{-3}$ | 1.86 | 2.09 | 2.33 | 2.57 | 2.83 | 3.41 |
| $H_{H_2S} \times 10^{-2}$ | 6.09 | 6.76 | 7.45 | 8.14 | 8.84 | 10.3 |

### 2.3 Enthalpy Data for Acid Gas-Amine Systems

The contribution to the liquid or vapour enthalpy of a component with negligible heat of mixing is readily determined using ideal vapour phase enthalpies, modified by latent heats of vapourization for the liquid phase. However, $H_2S$ and $CO_2$ have considerable heats of solution and few data are available on these.

On the basis of solubility data, Lee et al.[26,27,28] calculated approximate enthalpies of solution for $H_2S$ and $CO_2$ in both MEA and DEA. The values are tabulated in Appendix 1. In all cases the enthalpy of solution is strongly dependent on the acid gas loading, but information to date indicates no temperature dependence and relatively little dependence on solution normality. Kohl and Riesenfeld[24] have published single values for the enthalpies of solution of $H_2S$ and $CO_2$ in both MEA and DEA. The values are given in Appendix 1 and are in approximate agreement with those given by Lee et al.[26,27,28].

Pure component enthalpies can be obtained from the API Technical Data Book[1]. Latent heats for the amines are found in the Gas Conditioning Fact Book[11], and for water in Perry[6].

## 2.4 Numerical Solution of Stagewise Processes for Multicomponent Mixtures

### 2.4.1 Algorithms for Equilibrium Stage Calculations

Many algorithms exist for solving the nonlinear system of equations describing steady state conditions in separation devices. Most of these methods decouple the model equations, that is, the system of equations is split into two or more subsystems which are solved successively within the outer loop of an iteration procedure. Friday and Smith[10] have summarized many of the decoupled calculation methods in the light of six decisions that must be made to formulate a solution procedure. In a summary presented by Ishii[17], it is shown that decoupled methods are not reliable in that they have difficulty converging for certain types of problems. They are in addition less efficient and slower than methods that do not decouple the equations.

An alternative solution approach is to linearize the model equations and to solve them simultaneously. Although conceptually desirable, this approach may involve an enormous amount of computer storage and time. Thus few algorithms have been proposed, and these can become computationally unwieldy when composition dependent equilibrium and enthalpy data are employed.

Recently, Ishii[17] proposed a new algorithm that overcomes the practical difficulties of total linearization and results in a method that has proven to be both rapid and stable for a wide variety of problems[18]. His approach is to employ only those partial derivatives having a dominant effect on the solution in the linearized equations, thus reducing the matrix structures to forms that can be efficiently manipulated. This computational simplification in no way alters the rigour of the final results.

### 2.4.2 Stage Efficiencies

In the past much of the modelling of stagewise processes has involved ideal stages rather than real stages. An important refinement to the ideal stage model is then to incorporate some form of stage efficiency, particularly where the efficiency is vastly different for different components and on different stages.

Perhaps the most widely used efficiency is the Murphree[31] vapour stage efficiency, which is defined by equation (2-6):

$$E_{MV_{i,j}} = \frac{y_{i,j} - y_{i,j+1}}{K_{i,j}\, x_{i,j} - y_{i,j+1}} \qquad (2-6)$$

where $y_{i,j}$ and $y_{i,j+1}$ are the average compositions of the vapour leaving stages j and j+1 respectively, and $K_{i,j}\, x_{i,j}$ equals the vapour composition that would be in equilibrium with the liquid (of composition $x_{i,j}$) leaving stage j.

Simpler model equations than those obtained when using the Murphree efficiency can be achieved by employing a new efficiency defined by Holland[16]. The efficiency is termed a vapourization efficiency and is defined by equation (2-7):

$$y_{i,j} = e_{i,j}\, K_{i,j}\, x_{i,j} \qquad (2-7)$$

This definition assumes that the vapour solution is ideal and that thermal equilibrium exists between the leaving liquid and vapour streams.

It is possible to derive an expression for $e_{i,j}$ in terms of the mass transfer characteristics of the stage[16]. Consider a point z in the liquid pool on stage j, where z is the height above the tray. A component material balance gives:

$$V_j \frac{dy_i}{dz} + (K_{OG} a\, P)_{i,j}\, S(K_{i,j}\, x_{i,j} - y_i) = 0 \qquad (2\text{-}8)$$

where: V is the vapour flow rate, which is assumed to vary negligibly in the z direction (moles/hr)

$K_{OG}$ is the overall mass transfer coefficient (moles/ft$^2$ atm.hr)

a is the interfacial area per unit volume of column (ft$^2$/ft$^3$)

P is the pressure of stage j (atm)

S is the cross-sectional area of the column. (ft$^2$)

The vapour is assumed to mix totally between stages, but to be unmixed in passing through the liquid.

Separating the variables in equation (2-8) and integrating across the stage from z = 0 to $z = z_T$, the total depth of liquid, gives:

$$\int_{y_{i,j}}^{y_{i,j+1}} \frac{dy_i}{K_{i,j}\, x_{i,j} - y_i} = - \int_{0}^{z_T} \frac{(K_{OG} a\, P)_{i,j}}{V_j}\, S\, dz \tag{2-9}$$

This yields:

$$\ell n \left\{ \frac{K_{i,j}\, x_{i,j} - y_{i,j}}{K_{i,j}\, x_{i,j} - y_{i,j+1}} \right\} = - \frac{(K_{OG} a\, P)_{i,j}}{V_j}\, S\, z_T \tag{2-10}$$

and combining with equation (2-7) gives finally:

$$e_{i,j} = 1 - \exp\left\{ - \frac{(K_{OG} a\, P)_{i,j}}{V_j}\, S\, z_T \right\} \left[ 1 - \frac{y_{i,j+1}}{K_{i,j}\, x_{i,j}} \right] \tag{2-11}$$

This model assumes a well mixed stage. Modifications can be made to accommodate other mixing models[16].

Of the variables in equation (2-11), $K_{i,j}$, $x_{i,j}$, $y_{i,j+1}$, and $P_j$ are known from the profiles at each iteration, $(V_j/S)$ is the superficial gas velocity in the column and $z_T$, the outlet weir height, is known for a given column design. Thus $e_{i,j}$ is completely determined if $(K_{OG}a)_{i,j}$ can be estimated.

For the case of absorption combined with chemical reaction, $K_{OG}a$ is given by equation (2-12), where $k_g a$ and $k_L^o a$ are the individual gas and liquid phase resistances (in the absence of chemical reaction), H is the Henry's law coefficient and I is the enhancement factor.

$$\frac{1}{K_{OG}a} = \frac{1}{k_g a} + \frac{H}{Ik_L^o a} \qquad (2\text{-}12)$$

The enhancement factor is a measure of how much the rate of absorption is increased by the presence of chemical reaction, and it can be expressed as a function of the reaction rate for a given reaction regime[2]. For example, the penetration theory gives, for the instantaneous reaction regime[2],

$$I = \left(1 + \frac{D_2}{D_1}\frac{b_o}{q c'_o}\right) \Big/ \sqrt{\frac{D_2}{D_1}} \qquad (2\text{-}13)$$

## 2.5 Stage Efficiencies for Amine Units

Little work has been published on efforts to assign values to efficiencies in amine systems. Kohl[23] studied the absorption of $CO_2$ into MEA solutions. He calculated Murphree vapour stage efficiencies of between 8 and 25%, the low values indicating that the liquid film is controlling. Rowland and Grens[39] found a wide range of efficiency existed over a $CO_2$-MEA absorber. Their values were calculated from a fundamental approach, using constant values for $k_g a$, $k_L a$ and the liquid holdup, and ranged from 67% at the top to less than 5% at the bottom of the absorber.

Kohl and Riesenfeld[24] have published a correlation for $K_{OG}a$ for the absorption of $CO_2$ in MEA solutions. The correlation comes from a review of the available data and strictly applies only to a limited range of conditions and to absorption of $CO_2$ in the absence of $H_2S$. The expression is[24]:

$$K_{OG}a = (\frac{V}{z_T}) 1.2\text{x}10^{-4}/\mu^{0.68}[1+1.2(0.5 - X_{CO_2}) m\ e^{(.0067T-3.4p)}] \tag{2-14}$$

where: $K_{OG}a$ = overall mass transfer coefficient lb moles / (hr.ft$^3$.atm)

$V$ = actual gas volume (ft$^3$ / hr.ft$^2$ tray)

$z_T$ = height of contact zone (ft)

$\mu$ = viscosity, (cp)

$X_{CO_2}$ = concentration of $CO_2$ in solution (moles/mole MEA)

$m$ = amine concentration in solution (g moles/ℓ)

$T$ = temperature (°F)

$p$ = partial pressure (atm)

If the temperature is above 125°F, T in equation (2-14) is replaced by 250-T[23].

Relatively few studies on $H_2S$ absorption in amine solutions have been published, and no correlations such as equation (2-14) are available. However, $K_{OG}a$ could be estimated from fundamental rate data and equation (2-12). Both Astarita[2] and Danckwerts[7] suggest that $H_2S$ absorption occurs in the instantaneous reaction regime for the majority of conditions in an amine system. For the simultaneous absorption of $H_2S$ and $CO_2$, Danckwerts and Sharma[8] suggest the following expression for the enhancement factor, $I_1$, for $H_2S$ absorption, assuming the instantaneous reaction regime applies:

$$I_1 = \left[ 1 + \frac{\dfrac{[RNH_2]}{2c'_{o,1}} \dfrac{D_3}{D_1}}{1 + \dfrac{2c'_{o,2}}{c'_{o,1}} \dfrac{D_2}{D_1}} \right] \Bigg/ \sqrt{\frac{D_3}{D_1}} \qquad (2\text{-}15)$$

where: subscripts 1,2,3 refer to $H_2S$, $CO_2$ and MEA respectively.

$c'_{o,i}$ = solubility of i

$D_i$ = diffusivity of i

Instead of using equation (2-14), $K_{OG}a$ for $CO_2$ absorption could be calculated from equation (2-12) using the assumption that the reaction is fast regime[2]. In this case the liquid phase coefficient is given by:

$$k_L = Ik_L^o = \sqrt{k_1 D b_o} \qquad (2\text{-}16)$$

where $k_1$ is the pseudo first order rate constant for the reaction

$$CO_2 + 2RNH_2 \overset{k_1}{\rightleftharpoons} RNHCOO^- + RNH_3^+ \qquad (2\text{-}17)$$

In general the limited rate data available on amine systems makes a rigorous determination of stage efficiencies difficult.

## 2.6 Multicolumn Calculations

In most process flowsheet configurations there are a number of recycle streams. Prior to the development of digital computers, these streams made the closure of material balances around a process a job requiring perhaps man-weeks of effort. As computers came into widespread usage, various methods[32,33,37,38] were developed to perform the required iterative calculations far more speedily. Because methods of performing detailed equilibrium stage calculations had not been developed at that stage, each separation device or reaction unit within the system had to be treated in a simplified "black-box" fashion. Therefore, a split was approximated for each component around each device. Such a simplification made the solutions obtained far from rigorous.

More recently a few authors have published methods that solve rigorously the equilibrium stage equations in a system of separation devices. Most of these methods are extensions of previous algorithms developed to handle single columns, and the majority still employ a procedure that decouples the effect of some of the variables.

The "Theta method" has been applied to a number of linked column problems. Initially Tomme and Holland[42] applied the technique to a two column system. They termed the convergence method for systems the "capital" Theta method. A generalization of this procedure was presented by Nartker, Srygley and Holland[34]. Individual units within the system may be any of the conventional separation devices (absorber, reboiled absorber or distillation column) or a special type (mixer, proportional divider, flash unit). The general procedure is based on the calculational procedures for a single column, with the additional use of so-called system thetas, which force simultaneous convergence on all columns in the system. The $K_b$-method[15] was used to determine stage temperatures, and the constant composition and Q methods[15] to determine total flow rates. These produced a stable calculational procedure, although the number of iterations increased whenever side heaters or coolers had to be introduced according to the Q method.

Later Billingsley[3] presented a simplified formulation of the above procedure. It involves only the theta correction factors used in formulating the equations for a single column, thus making the system thetas redundant. In addition Billingsley notes that in certain cases matrices in the general procedure of Nartker et al.[34] may be nearly singular, in which case gross errors would occur in the material balance around the system. He presents a modification to the equations used which eliminates the difficulty.

Petryschuk and Johnson[36] employed the method of Nartker et al.[34] in the simulation of a complete light ends recovery system. They utilized two other calculation methods - a system block-relaxation method and a sequential iterative method. For a particular recycle loop in the light ends system, a combination of the system theta-method and the block-relaxation method was found to be the superior technique. This combination was up to ten times as fast as the pure block-relaxation method, illustrating the asymptotic approach of the latter to the final solution.

Jelinek et al.[20] found the block-relaxation method superior to the sequential iterative method. The off-diagonal elements in the material balance matrix, which arise from recycle streams between columns, were handled by a special modification of Gaussian elimination.

All of the above methods decouple the material balances from the energy balances, and most would still perform bubble point calculations for the stage temperatures. The desirability of simultaneous solution of all equations has been recognised for some time, but it is only recently that methods have appeared that successfully do this. At present, Harclerode and Gentry[14] are the only authors to have published the application of such a method to a system of columns.

The algorithm is an extension of Gentry's earlier method[12]. In the multiple column case, the matrix equations involve matrices with a limited number of rows and columns that are completely full. Special matrix methods and a modified form of Gaussian elimination are used in the reduction of the matrices to a form where back substitution will yield a solution. Both procedures are specially designed to increase the efficiency of the matrix manipulations and to decrease computing time. One restriction on the method is that the specifications for a column must be symmetrical, i.e. the specification must apply to the same stage as the equation it replaces. The complexity of the matrix manipulations increases markedly when composition dependent equilibrium and enthalpy data are employed.

## 3. MODELLING AMINE CONTACTORS AND REGENERATORS

### 3.1 Stage Model

A generalized stage model is shown as Figure 2. This model can represent any of the usual separation devices, but in the present context will refer primarily to amine absorbers (contactors) or regenerators.

The steady state model equations for any stage j, and component i may be represented as follows:

(1) Phase Relationships:

$$y_{i,j} = e_{i,j} K_{i,j} x_{i,j} \tag{3-1}$$

These reduce to equilibrium relationships if the efficiency factors, $e_{i,j}$, are all equal to unity.

(2) Component Material Balances:

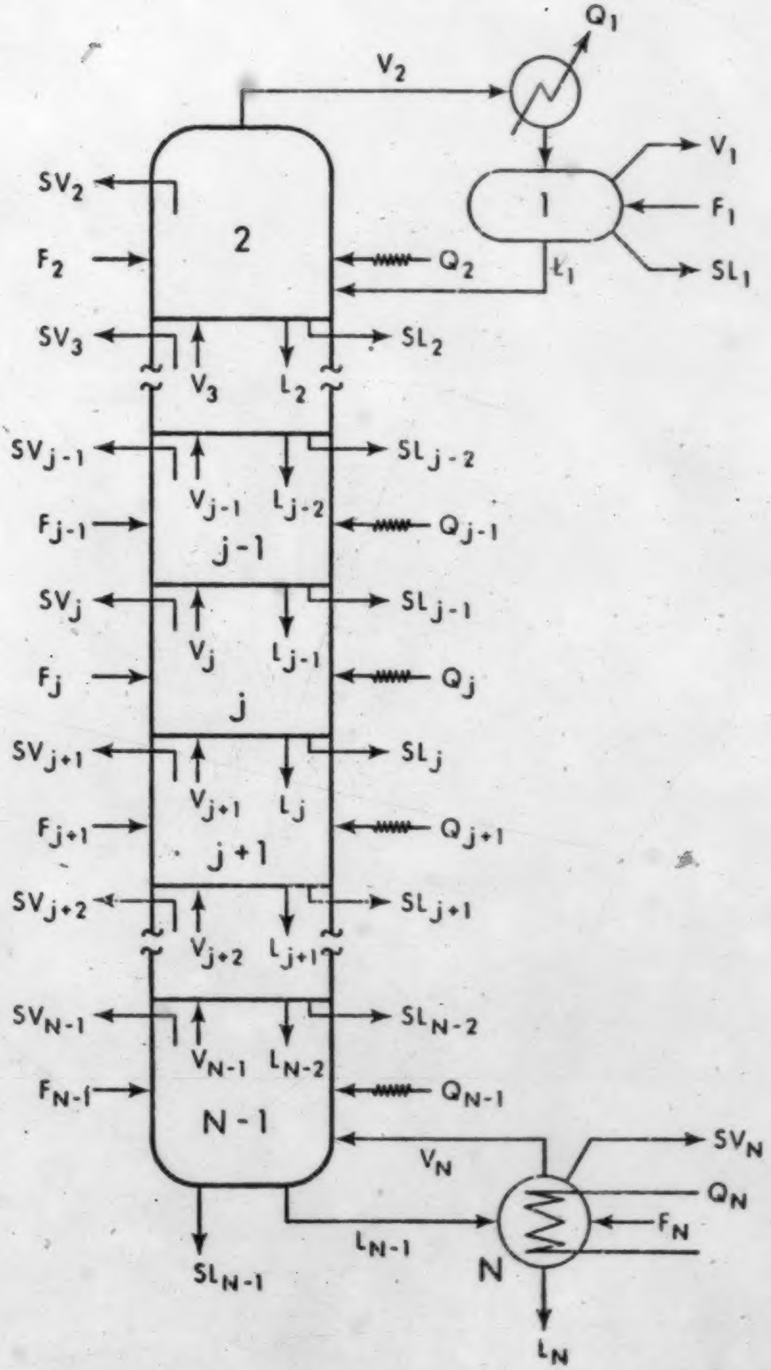
$$F_j z_{i,j} + L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} - (L_j+SL_j) x_{i,j} - (V_j+SV_j) y_{i,j} \equiv c_{i,j} \tag{3-2}$$

(3) Energy Balance:

$$F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} - (L_j+SL_j) h_j - (V_j+SV_j) H_j \equiv E_j \tag{3-3}$$

(4) Summation Equation:

$$\sum_{i=1}^{NCP} x_{i,j} - 1.0 \equiv S_j \quad \text{or} \quad \sum_{i=1}^{NCP} y_{i,j} - 1.0 \equiv S_j \tag{3-4}$$



$Q_1$
$V_2$
$V_1$
1
$F_1$
$SL_1$
$SV_2$
2
$F_2$
$Q_2$
$L_1$
$SV_3$
$V_3$
$L_2$
$SL_2$
$SV_{j-1}$
$SL_{j-2}$
$V_{j-1}$
$L_{j-2}$
$F_{j-1}$
j-1
$Q_{j-1}$
$SV_j$
$SL_{j-1}$
$V_j$
$L_{j-1}$
$F_j$
j
$Q_j$
$SV_{j+1}$
$SL_j$
$V_{j+1}$
$L_j$
$F_{j+1}$
j+1
$Q_{j+1}$
$SV_{j+2}$
$SL_{j+1}$
$V_{j+2}$
$L_{j+1}$
$SV_{N-1}$
$SL_{N-2}$
$V_{N-1}$
$L_{N-2}$
$F_{N-1}$
N-1
$Q_{N-1}$
$V_N$
$SV_N$
$Q_N$
$F_N$
$L_{N-1}$
N
$SL_{N-1}$
$L_N$

FIGURE 2: GENERALIZED STAGE MODEL

(5) Overall Material Balance:

$$F_j + L_{j-1} + V_{j+1} - (L_j+SL_j) - (V_j+SV_j) \equiv M_j \tag{3-5}$$

Normally equations (3-1) and (3-2) are combined to give:

$$\begin{aligned} &F_j\, z_{i,j} + L_{j-1}\, x_{i,j} + V_{j+1}\, e_{i,j+1}\, K_{i,j+1},\, x_{i,j+1} \\ &\quad - (L_j+SL_j)\, x_{i,j} - (V_j+SV_j)\, e_{i,j}\, K_{i,j}\, x_{i,j} \\ &\quad \equiv c_{i,j} \end{aligned} \tag{3-6}$$

The following quantities must be specified in order to match the number of unknowns with the number of independent equations.

(i) the total number of stages

(ii) the pressure at each stage

(iii) the location, total rate, composition and condition of each feed

(iv) the location and total quantity of each side stream (liquid or vapour)

(v) the location and heat duty of any intercoolers or heaters (including condenser and reboiler)

(vi) the values of the vapourization efficiencies.

It should be noted that any of the above specifications may be replaced by an equivalent specification involving another variable. In particular, for regenerator problems it is often of interest to specify the condenser temperature in place of the condenser load.

Values of the vapourization efficiencies may be supplied as constants at the initialization phase of the computer program, or a value may be calculated at each iteration from the current profiles and a knowledge of the dynamics of the tray in question (see equation (2-11)).

### 3.1.1 Solution Procedure

A solution to the model equations is obtained when a set of values of the temperatures, $T_j$'s, the liquid and vapour flow rates, $L_j$'s, and $V_j$'s, and the phase compositions, $x_{i,j}$'s and $y_{i,j}$'s, is found which makes all the $M_j$, $c_{i,j}$, $E_j$ and $S_j$ equal to zero.

The method of solution which forms the basis of this thesis is that developed by Y. Ishii[17]. It is essentially a modified Newton-Raphson method, and employs the Taylor approximation procedure in the linearization of the equations.

For the purpose of linearization the $e_{i,j}$ are assumed independent of temperature and composition.

The linearized equations are:

(1) Component Material Balances:

$$L_{j-1}\,\Delta x_{i,j-1} - \left[(L_j+SL_j)+(V_j+SV_j)\,e_{i,j}\,(K_{i,j}+x_{i,j}\,\frac{\partial K_{i,j}}{\partial x_{i,j}})\right]\Delta x_{i,j}$$

$$+\,V_{j+1}\,e_{i,j+1}\,(K_{i,j+1}+x_{i,j+1}\,\frac{\partial K_{i,j+1}}{\partial x_{i,j+1}})\,\Delta x_{i,j+1}$$

$$-\,(V_j+SV_j)\,e_{i,j}\,x_{i,j}\,\frac{\partial K_{i,j}}{\partial T_j}\,\Delta T_j$$

$$+\,V_{j+1}\,e_{i,j+1}\,x_{i,j+1}\,\frac{\partial K_{i,j+1}}{\partial T_{j+1}}\,\Delta T_{j+1}$$

$$+\,\Delta L_{j-1}\,x_{i,j-1} - \Delta L_j\,x_{i,j} - \Delta V_j\,y_{i,j}$$

$$+\,\Delta V_{j+1}\,y_{i,j+1} = -c_{i,j} \qquad (3\text{-}7)$$

(2) Energy Balance:

$$L_{j-1}\,\frac{\partial h_{j-1}}{\partial T_{j-1}}\,\Delta T_{j-1} - \left[(L_j+SL_j)\,\frac{\partial h_j}{\partial T_j} + (V_j+SV_j)\,\frac{\partial H_j}{\partial T_j}\right]\Delta T_j$$

$$+\,V_{j+1}\,\frac{\partial H_{j+1}}{\partial T_{j+1}}\,\Delta T_{j+1} + \Delta L_{j-1}\,h_{j-1} - \Delta L_j\,h_j$$

$$-\,\Delta V_j\,H_j + \Delta V_{j+1}\,H_{j+1} = -E_j \qquad (3\text{-}8)$$

(3) Overall Material Balance:

$$\Delta L_{j-1} + \Delta V_{j+1} - \Delta L_j - \Delta V_j = -M_j \qquad (3\text{-}9)$$

(4) Summation Equation:

$$\sum_{i=1}^{NCP} \Delta x_{i,j} = -S_j \qquad (3\text{-}10)$$

It is readily seen that all equations apart from the component material balance equations are identical to the equilibrium case, and thus no different handling methods are necessary in formulating a solution. The solution procedure is the same as that described by Ishii[17]. Iterative calculations are continued until a suitable convergence criterion[17] is satisfied.

### 3.1.2 Initial Assumptions

To begin the iterative solution procedure it is necessary to have initial values of the $V_j$'s, $L_j$'s, $T_j$'s, $x_{i,j}$'s and $y_{i,j}$'s. A knowledge of the operating characteristics of amine units can be employed to do this.

(a) Vapour Flow Rates:

For a contactor all the $V_j$'s can be set equal to the quantity of hydrocarbons, nitrogen and hydrogen in the sour gas. This is equivalent to assuming most of the absorption occurs on the bottom stage. In a regenerator, the top vapour product can be approximated by the quantity of acid gas, hydrogen, nitrogen and light hydrocarbons in the feed to the regenerator. The initial reflux ratio is usually set at 2, and this then gives $V_2$. The other $V_j$'s are then increased down the column, tapering off to almost constant molar flowrates in the bottom half.

(b) Liquid Flow Rates:

Once the $V_j$'s have been estimated, $L_j$'s are obtained from equation (3-5), with $M_j = 0$.

(c) Temperature:

For the contactor a linear interpolation between the top and bottom stage temperatures is generally sufficient. The temperature of the top stage can be set equal to the lean amine feed temperature. The bottom stage temperature is more difficult to estimate and depends on the quantity of acid gas being absorbed. If necessary approximate values of the enthalpy of solution of $H_2S$ and $CO_2$ can be used to calculate the expected temperature rise in the liquid.

For the regenerator, the condenser temperature is specified and the reboiler temperature will normally be about 255°F. The temperature of the feed stage (normally the second) can be approximated as 30-40°F above the temperature of the feed. A linear interpolation between this temperature and the reboiler is then used. If the feed stage is not the second stage, then stages between the condenser and the feed can assume the feed stage temperature.

(d) Liquid Compositions

For the Contactor,

(i) the bottom stage composition for $H_2S$ and $CO_2$ is obtained by assuming that all the acid gas, in all feeds, is absorbed into the rich amine. On other stages the respective compositions are equated to the lean amine composition.

(ii) MEA/DEA and water are assumed to remain solely in the liquid.

(iii) other components in the feed, such as hydrogen, nitrogen and light hydrocarbons, are assumed to remain solely in the vapour.

For the Regenerator,

(i) in the condenser the compositions are set equal to the following, where subscripts 1,2, 3, and 4 refer to $H_2S$, $CO_2$, MEA/DEA and $H_2O$ respectively:

$x_1 = .001, \quad x_2 = .0002, \quad x_3 = .006,$

$x_4 = .9928, \quad x_i = .001\, Z_i, \quad i = 5 \rightarrow NCP$

where $z_i$ is the composition in the rich amine feed. The same values apply for stages between the condenser and the feed stage.

(ii) on the feed stage $H_2S$, $CO_2$, MEA/DEA and $H_2O$ are assigned their respective feed compositions. For other components, their overall composition in the feed is reduced by a factor of 1000 to give the liquid phase compositions.

(iii) for stages between the feed and the reboiler, the $H_2S$ and $CO_2$ compositions are linearly interpolated to zero at a fictional stage one below the reboiler (to give a nonzero composition in the reboiler), MEA/DEA and water are assumed to remain solely in the liquid, and other components have their compositions reduced by a factor of 10 on each successive stage.

### (e) Vapour Compositions

Once liquid phase compositions have been estimated and normalized, K-ratios can be determined. The $y_{i,j}$'s are then given by equation (3-1).

## 3.2 Determination of Equilibrium K-ratios

The modified model of Klyamer et al.[22], as derived by Nasir[35], was used to predict the partial pressures of $H_2S$ and $CO_2$ (see equations 2-4 and 2-5). The equilibrium ratios are then given by equation (3-11), where i represents either $H_2S$ or $CO_2$.

$$K_i = \frac{P_i}{P_T \, x_i} \tag{3-11}$$

For the condenser, where there is a dilute solution of the acid gas components in water, the K ratios are determined via the Henry's Law coefficients for $H_2S$ and $CO_2$, as tabulated in Table 1. The temperature range of the data in the table covers the normal range of condenser temperatures.

With only a few data points it was deemed sufficiently accurate to use Lagrange interpolating polynomials. These were made to pass through the data points at temperatures of 30,40,50 and 60°C, and then slight adjustments made to the coefficients to ensure a good match at temperatures of 35 and 45°C. A third order polynomial was chosen as this produces a curve with a small oscillatory nature.

The equations for the Henry's Law coefficients are then:

(1) For $H_2S$

$$\begin{aligned} H = {} & 0.1717\ (T-30)(T-40)(T-50) \\ & -0.442\ (T-30)(T-40)(T-60) \\ & +0.3725\ (T-30)(T-50)(T-60) \\ & -0.1015\ (T-40)(T-50)(T-60) \end{aligned} \tag{3-12}$$

(2) For $CO_2$

$$\begin{aligned} H = {} & 0.568\ (T-30)(T-40)(T-50) \\ & -1.415\ (T-30)(T-40)(T-60) \\ & +1.165\ (T-30)(T-50)(T-60) \\ & -0.310\ (T-40)(T-50)(T-60) \end{aligned} \tag{3-13}$$

Finally the K-values are given by the equation

$$K_i = \frac{H_i}{P} \tag{3-14}$$

where: P is the condenser pressure in atmospheres
i refers to either $H_2S$ or $CO_2$.

For other components the Henry's Law coefficients have been curvefitted as a function of temperature. Some of these fits are quite approximate because of the paucity of data for the solubility of hydrocarbons in amine solutions. For simplicity all fractions higher than $C_6$ are lumped together.

Raoult's Law is employed to give the partial pressure, and thus the equilibrium K-ratios are given by equation (3-15).

$$K_i = \frac{H_i}{P_T} \qquad i = 5 \rightarrow NCP \qquad (3\text{-}15)$$

where: $P_T$ is in mm $H_g$

$H_i$ is in mm $H_g$/mole fraction.

### 3.3 Determination of Enthalpies

The molar enthalpy of component i as an ideal gas, $H_i^o$, is given by the following cubic equation in temperature, $^oR$. The coefficients are taken from the API Technical Data Book[1] and are given in Appendix 2.

$$H_i^o = \{A_i(T/100) + B_i(T/100)^2 + C_i(T/100)^3 + D_i(100/T) + E_i\}\ XM_i \qquad (3\text{-}16)$$

The molar enthalpy of the gas phase is then given by equation (3-17)

$$H = \sum_{i=1}^{NCP} y_i\ H_i^o \qquad (3\text{-}17)$$

For non-volatile components, namely MEA/DEA and water, the latent heat of vapourization has been correlated as a quadratic in temperature, °R.

$$H_{vap,i} = \{AL_i + BL_i\ T + CL_i\ T^2\}\ XM_i \qquad (3\text{-}18)$$

The coefficients are given in Appendix 2.

The enthalpy of the liquid phase is given by:

$$h = \sum_{i=1}^{NCP} x_i \left(H_i^O - H_{vap,i} + \Delta H_{sol}\right) \qquad (3\text{-}19)$$

$\Delta H_{sol}$ is the enthalpy of solution of the acid gas components. Values are tabulated in Appendix 1.

## 3.4 Development of Partial Derivatives

Linearization of the model equations introduces a set of partial derivatives that must be evaluated either numerically or analytically at each iteration. In accordance with the findings of Ishii[17], only those partials with a dominant effect on the solution need be evaluated, namely

$$\frac{\partial K_{i,j}}{\partial T_j}, \quad \frac{\partial K_{i,j}}{\partial x_{i,j}}, \quad \frac{\partial H_j}{\partial T_j} \text{ and } \frac{\partial h_j}{\partial T_j}$$

The K-ratios for components other than $H_2S$ and $CO_2$ are given by equation (3-15). Then the partial derivatives with respect to T and x are:

$$\frac{\partial K_{i,j}}{\partial T_j} = \left\{\frac{1}{P_T}\frac{\partial H_i}{\partial T}\right\}_j \qquad (3\text{-}20)$$

$$\frac{\partial K_{i,j}}{\partial x_{i,j}} = 0 \qquad (3\text{-}21)$$

For $H_2S$ and $CO_2$, $\partial K_{i,j}/\partial T_j$ was evaluated numerically using a step size of 1°F.

$\frac{\partial K_{i,j}}{\partial x_{i,j}}$ for these two components can be derived analytically as follows:

The implicit expressions for the partial pressures of $H_2S$ and $CO_2$, are given by equations (2-4) and (2-5) as:

$$P_{H_2S} = \frac{K_W}{K_i \; K_{1c} \; H_{H_2S}} \cdot \frac{\gamma 2}{a\alpha} \cdot \frac{A(A+B)}{(m-z-A-B)} \qquad (2\text{-}4)$$

$$P_{CO_2} = \frac{1}{K_m} \cdot \frac{\gamma^2}{a^2\alpha^2} \cdot \frac{z(A+B)}{(m-z-A-B)^2} \qquad (2\text{-}5)$$

Then using equation (3-11) with each of (2-4) and (2-5) in turn, and rearranging yields:

$$(K_i \; K_{1c} \; P_T \; H_{H_2S} \; a\alpha) \; K_{H_2S} \; x_{H_2S} \; (m-z-A-B)$$
$$- K_W \, \gamma^2 \, A(A+B) = 0 \qquad (3\text{-}22)$$

$$(K_m \; P_T \; a^2\alpha^2) \; K_{CO_2} \; x_{CO_2} \; (m-z-A-B)^2$$
$$- \gamma^2 \, z(A+B) = 0 \qquad (3\text{-}23)$$

Both of these equations are of the form

$$F(K_j, x_j) = \text{constant}$$

where j represents $H_2S$ or $CO_2$.

Then the partial derivative of $K_j$ with respect to $x_j$ is given by

$$\frac{\partial K_j}{\partial x_j} = \frac{-\left(\frac{\partial F}{\partial x_j}\right)_{K_j}}{\left(\frac{\partial F}{\partial K_j}\right)_{x_j}} \tag{3-24}$$

(A) For $H_2S$ (subscript 1 $\equiv H_2S$)

$$\text{(i)}\quad \left(\frac{\partial F}{\partial x_1}\right)_{K_1} = K_i\, K_{1c}\, P_T\, H_1\, a\, K_1 \left[\alpha(m-z-A-B) + x_1\{(m-z-A-B)\frac{\partial \alpha}{\partial x_1} - \alpha \frac{\partial A}{\partial x_1}\}\right] - K_W\left[\gamma^2(2A+B)\frac{\partial A}{\partial x_1} + 2\gamma A(A+B)\frac{\partial \gamma}{\partial x_1}\right] \tag{3-25}$$

$$\text{(ii)}\quad \left(\frac{\partial F}{\partial K_1}\right)_{x_1} = K_i\, K_{1c}\, P_T\, H_1\, a\alpha\, x_1 \left[(m-z-A-B) - K_1 \frac{\partial A}{\partial K_1}\right] - K_W\, \gamma^2\, \{2A+B\} \frac{\partial A}{\partial K_1} \tag{3-26}$$

The partial derivatives required to evaluate $\partial F/\partial x_1$ and $\partial F/\partial K_1$ are given in Appendix 3.

(B) For $CO_2$ (subscript $2 \equiv CO_2$)

(i)
$$\left(\frac{\partial F}{\partial x_2}\right)_{K_2} = K_M P_T a^2 K_2 \left[ \alpha^2 (m-z-A-B)^2 + x_2 (m-z-A-B)^2 \left(2\alpha \frac{\partial \alpha}{\partial x_2}\right) + 2x_2 (m-z-A-B)\alpha^2 \left(- \frac{\partial z}{\partial x_2} - \frac{\partial B}{\partial x_2}\right)\right] - 2\gamma z (A+B) \frac{\partial \gamma}{\partial x_2} - \gamma^2 z \frac{\partial B}{\partial x_2} - \gamma^2 (A+B) \frac{\partial z}{\partial x_2} \quad (3\text{-}27)$$

(ii)
$$\left(\frac{\partial F}{\partial K_2}\right)_{x_2} = K_M P_T a^2 \alpha^2 x_2 \left[ (m-z-A-B)^2 + 2K_2 (m-z-A-B)\left(-\frac{\partial z}{\partial K_2} - \frac{\partial B}{\partial K_2}\right)\right] - \gamma^2 \left\{ (A+B) \frac{\partial z}{\partial K_2} + z \frac{\partial B}{\partial K_2}\right\} \quad (3\text{-}28)$$

where the required partial derivatives are given in Appendix 3.

In the special case of the condenser of the regenerator the partial derivatives are computed by differentiating equations (3-12) and (3-13). Thus:

$$\frac{\partial K_{i,j}}{\partial T_j} = \begin{array}{l} (15.84 - .138T + .0021T^2) / 1.8\,P \text{ for } H_2S \\ (74.1 - 1.62T + .024T^2) / 1.8\,P \text{ for } CO_2 \end{array} \qquad (3\text{-}29)$$

$$\frac{\partial K_{i,j}}{\partial x_{i,j}} = 0 \qquad (3\text{-}30)$$

$\frac{\partial H}{\partial T}$, $\frac{\partial h}{\partial T}$ are expressed as follows:

$$\frac{\partial H}{\partial T} = \sum_{i=1}^{NCP} y_i \frac{\partial H_i^o}{\partial T} \qquad (3\text{-}31)$$

$$\frac{\partial h}{\partial T} = \sum_{i=1}^{NCP} x_i \left\{\frac{\partial H_i^o}{\partial T} - \frac{\partial H_{vap,i}}{\partial T}\right\} \qquad (3\text{-}32)$$

where:

$$\frac{\partial H_i^o}{\partial T} = \{A_i + 2B_i(T/100) + 3C_i(T/100)^2 - D_i(100/T)^2\} \frac{XM_i}{100} \qquad (3\text{-}33)$$

$$\frac{\partial H_{vap,i}}{\partial T} = (BL_i + 2CL_iT)\ XM_i \qquad (3\text{-}34)$$

In the region of low acid gas loadings empirical corrections are added to the expressions for the activity coefficient, $\gamma$, and to the final expressions for the partial pressures of $H_2S$ and $CO_2$. The dependence of these corrections on liquid composition or temperature is expected to be slight and therefore no corrections are made to the partial derivatives.

# 4. APPLICATION OF THE MODEL TO THE DESIGN OF AMINE UNITS

The intention of this chapter is to demonstrate how the computational model may be used in the design of contactors and regenerators. Four test problems, using both MEA and DEA as solvents, are presented and the results obtained with two different data correlations are given. Other uses of the model are indicated, with detailed attention being focussed on evaluating the relationship between the lean amine residuals of the acid gas components and the sweet gas $H_2S$ composition. Finally, details are given of one method of predicting the vapourization efficiencies for $H_2S$ and $CO_2$ in amine units.

## 4.1 Test Problems

The following four problems are typical of amine contactors and regenerators operating in natural gas processing plants.

**Example Problem No. 1** - MEA Contactor

The problem specifications and initial assumptions are as follows:

## Compositions Of Entering Streams

| Component | Sour Gas (moles/time) | Semilean Amine (moles/time) | Lean Amine (moles/time) |
|---|---|---|---|
| $H_2S$ | 18.7 | 54.3 | 1.28 |
| $CO_2$ | 2.95 | 6.3 | 1.57 |
| MEA | - | 250.0 | 62.05 |
| Water | 5.91 | 2550.0 | 630.93 |
| hydrogen | 629.97 | - | - |
| nitrogen | 29.53 | - | - |
| methane | 781.55 | - | - |
| ethane | 354.36 | 0.16 | - |
| propane | 124.02 | 0.42 | - |
| n-butane | 1.97 | - | - |
| i-butane | 19.69 | - | - |

The sour gas is a little over 1% total acid gas, and both lean and semilean amine streams are 25 weight percent. The lean amine contains 50 grains per gallon (gr/gal) of both $H_2S$ and $CO_2$, while the semilean amine contains 2200 gr/gal $H_2S$ and 200 gr/gal $CO_2$.

Number of ideal stages = 20

Feed temperatures:

Sour gas = 95°F
Semilean amine = 120°F
Lean amine = 100°F

Semilean amine enters stage 4.

Column pressure = 150 psia.

### Initial Assumptions

| Stage No. | Temperature(°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 110 | 1960 |
| 2→20 | 120 | 1960 |

## Example Problem No. 2 - DEA Contactor

This problem corresponds to medium pressure DEA contactors operating in Alberta. Specifications and initial assumptions are:

### Compositions Of Entering Streams

| Component | Sour Gas (moles/day) | Semilean Amine (moles/day) | Lean Amine (moles/day) |
|---|---|---|---|
| $H_2S$ | 6948.0 | 290.5 | 36.3 |
| $CO_2$ | 868.4 | 140.25 | 28.1 |
| →DEA | - | 8147.5 | 5415.0 |
| $H_2O$ | - | 154,650.0 | 70,260.0 |
| methane* | 21,130.6 | - | - |

---

* because the relative compositions of the light hydrocarbon components were unknown, all such components were considered as methane for convenience.

These compositions correspond to 24% $H_2S$ and 3% $CO_2$ in the sour gas, a 31 weight percent DEA lean amine solution with 40 grains per gallon each of $H_2S$ and $CO_2$, and a 23.6 weight percent DEA semilean amine solution, containing 160 grains per gallon $H_2S$ and 100 grains per gallon $CO_2$. The flowrates of lean and semilean amine are respectively 150 and 300 gallons per minute.

Number of ideal stages = 4

Feed temperatures:

Sour gas = 100°F
Semilean amine = 145°F
Lean amine = 135°F

Semilean amine enters stage 2

Column pressure = 712 psia.

## Initial Assumptions

| Stage No. | Temperature(°F) | Vapour Rate (moles/day) |
|---|---|---|
| 1 | 135 | 21,131 |
| 2 | 140 | 21,131 |
| 3 | 145 | 21,131 |
| 4 | 150 | 21,131 |

## Example Problem No. 3 - MEA Regenerator

The problem specifications and initial assumptions are:

### Feed Composition

| Component | Feed (moles/time) |
|---|---|
| $H_2S$ | 1140.2 |
| $CO_2$ | 101.8 |
| MEA | 3220.0 |
| $H_2O$ | 32730.0 |
| $H_2$ | 0.67 |
| $N_2$ | 0.04 |
| $CH_4$ | 0.57 |
| $C_2H_6$ | 0.32 |
| $C_3H_8$ | 0.34 |

Number of ideal stages = 14

Feed stage number = 2

Feed conditions: temperature = 200°F

Pressure = 100 psia

Column pressure = 28 psia

Pressure drop per stage = 0.33 psia

Condenser: temperature = 120°F

Pressure = 27 psia

Reboiler duty = 114.11 MM BTU/time.

The rich amine is 25 weight percent MEA containing about 3650 gr/gal $H_2S$ and 250 gr/gal $CO_2$. The reboiler duty corresponds to 1.3 lbs. of 55 psia steam per gallon of amine solution.

Initial Assumptions

| Stage No. | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 120 | 1140 |
| 2 | 230 | 3420 |
| 3 | 240 | 5000 |
| 4 | 242 | 5100 |
| 5 | 244 | 5200 |
| 6 | 246 | 5300 |
| 7 | 248 | 5400 |
| 8 | 250 | 5500 |
| 9 | 252 | 5600 |
| 10 | 254 | 5700 |
| 11 | 256 | 5800 |
| 12 | 258 | 5900 |
| 13 | 260 | 6000 |
| 14 | 262 | 6100 |

Estimated reflux ratio = 2.0.

## Example Problem No. 4 - DEA Regenerator

The problem specifications and initial assumptions are:

### Feed Composition

| Component | Feed (moles/time) |
|---|---|
| $H_2S$ | 37.82 |
| $CO_2$ | 123.71 |
| DEA | 290.88 |
| $H_2O$ | 6012.4 |
| $CH_4$ | 0.43 |
| $C_2H_6$ | 0.03 |
| $C_3H_8$ | 0.01 |

The DEA solution is 22 weight percent and the reboiler duty corresponds to approximately 1 lb. of 55 psia steam per gallon of amine solution.

Number of ideal stages = 14
Feed stage number = 2
Feed conditions: temperature = 180°F
Pressure = 48 psia
Column pressure = 27 psia
Pressure drop per stage = 0.33 psia
Condenser: temperature = 100°F
pressure = 25 psia

Reboiler duty = 16.171 MM BTU/time

Vapourization efficiencies:

$H_2S = 0.7$, $CO_2 = 0.3$ } on all stages

## Initial Assumptions

| Stage No. | Temperature(°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 100 | 160 |
| 2 | 220 | 400 |
| 3 | 232 | 700 |
| 4 | 234 | 850 |
| 5 | 236 | 900 |
| 6 | 238 | 905 |
| 7 | 240 | 910 |
| 8 | 242 | 915 |
| 9 | 244 | 920 |
| 10 | 246 | 925 |
| 11 | 248 | 930 |
| 12 | 250 | 935 |
| 13 | 252 | 940 |
| 14 | 254 | 945 |

Estimated reflux ratio = 1.5 .

## 4.2. Discussion of Test Problems

The detailed computer printouts for the test problems are found in Appendix 4. Two different data correlations were used for each problem:

(a) Nasir's[35] modification of the work of Klyamer et al.[22]

(b) the correlation supplied by AMOCO[25]

Table 2 lists a comparison of the number of iterations and CPU times required for each correlation. The computer used was an IBM 360/67. In general fewer iterations are needed when employing the AMOCO correlation, but more CPU seconds per iteration.

TABLE 2: NUMBER OF ITERATIONS AND CPU TIMES REQUIRED FOR TEST PROBLEMS FOR TWO DATA CORRELATIONS

| CORRELATION USED → <br> ↓ PROBLEM | NASIR | | AMOCO | |
|---|---|---|---|---|
| | NO. OF ITERATIONS | CPU TIME (SECONDS) | NO. OF ITERATIONS | CPU TIME (SECONDS) |
| 1 MEA Contactor | 6 | 17.2 | 6 | 17.7 |
| 2 DEA Contactor | 4 | 1.7 | 3 | 1.7 |
| 3 MEA Regenerator | 6 | 6.8 | 5 | 8.3 |
| 4 DEA Regenerator | 10 | 10.3 | 7 | 11.3 |

The latter is largely because in the AMOCO correlation a standard set of 18 components is used and this results in a number of redundant multiplications when any of the 18 are not present.

The different data correlations produce very different results. The comparative values of important design variables for each test problem are given in Table 3. It is obvious from the tabulated values that the results are highly sensitive to the data correlation used.

TABLE 3: COMPARISON OF THE VALUES OF IMPORTANT DESIGN VARIABLES.

| PROBLEM | VARIABLE | NASIR | AMOCO |
|---|---|---|---|
| MEA Regenerator | Reflux ratio | 1.87 | 1.79 |
| | Moles $H_2S$ in lean amine | 125.1 | 94.2 |
| | Moles $CO_2$ in lean amine | 59.3 | 84.3 |
| DEA Regenerator | Reflux ratio | 1.33 | 1.22 |
| | Moles $H_2S$ in lean amine | 2.69 | 0.47 |
| | Moles $CO_2$ in lean amine | 17.0 | 12.6 |
| MEA Contactor | ppm $H_2S$ in sweet gas | 10.14 | 15.82 |
| | ppm $CO_2$ in sweet gas | 0.09 | 0.22 |
| DEA Contactor | ppm $H_2S$ in sweet gas | 3.18* | 1.57 |
| | ppm $CO_2$ in sweet gas | 0.40* | 0.10 |

---

* not using empirical corrections to K-ratios at low acid gas loadings.

Nasir's correlation[35] lies closer to published experimental curves than do the other three correlations referenced in this work[21,22,25]. However, his correlation exhibits a limitation at very low acid gas loadings. Namely, the empirical corrections used to force the predicted solubilities to follow the trend of experimental curves for conditions found in the base of the regenerator, encounter a discontinuity at $x_{H_2S} = 0.0095$. This is the reason the empirical corrections were not applied in the DEA contactor problem. The discontinuity problem will be encountered when very low partial pressures are achieved in the sweet gas, and particularly in medium and high pressure contactors.

For a given data correlation, the model can be used to determine optimal values of variables that are important cost-wise, particularly the reboiler load and the amine circulation rate.

The reboiler load must be adequate to reduce the quantity of acid gas components in the regenerated amine to acceptably low levels. In addition the entering temperature of the rich amine feed can affect the amount of heat required. Often a hotter feed may significantly lower the reboiler load. The reflux ratio is also dependent on the reboiler load and may be found to exceed the rule-of-thumb criterion of being between 1.0 and 3.0, if too little, or too much, heat is supplied.

The amine circulation rate can be varied in order to obtain an acceptable $H_2S$ level in the sweet gas. The option of using a semilean stream can also be investigated using the model. This involves both the composition and quantity, and the entering stage, of the stream. For example, if problem 1 is repeated with 4 ideal stages (using Nasir's model) and the semilean enters on stage 3, the sweet gas contains 14 ppm $H_2S$. If instead the semilean enters on stage 2, the sweet gas contains 66 ppm $H_2S$.

Incorporating the vapourization efficiencies changes the results obtained. Problem 4 was run twice with a reboiler load of 17.0 MM BTU, and with vapourization efficiencies on all stages of:

(i) 1.0 for both $H_2S$ and $CO_2$

(ii) 0.7 for $H_2S$, 0.3 for $CO_2$

The calculated reflux ratios were respectively 0.95 and 1.70. In the ideal stage case 4.04 moles $H_2S$ and 7.71 moles $CO_2$ remained in the regenerated amine; for case (ii) there were 2.83 moles $H_2S$ and 16.59 moles $CO_2$. The next section illustrates how important accurate estimation of these residuals is in reaching an acceptable $H_2S$ level in the sweet gas.

Details of calculating vapourization efficiencies from fundamental rate data are considered in Section 4.4.

## 4.3 Dependence of Sweet Gas $H_2S$ Composition on Lean Amine Residuals.

The model can be used to obtain information on the relationship between the lean amine residual compositions of $H_2S$ and $CO_2$ and the composition of $H_2S$ in the sweetened gas. Figure 3 shows the results of such an investigation utilizing the model developed by Nasir[35]. In the figure ppm $H_2S$ in the sweet gas is plotted against grains of $H_2S$ per gallon of circulating lean amine solution, at various loadings of $CO_2$ in the lean amine (gr/gal).

The contactor used in the study had the following specifications:

Number of ideal stages = 10
Feed temperatures:
sour gas = 100°F
lean amine = 110°F
Column pressure = 500 psia

The sour gas was 20 percent total acid gas and the acid gas loading in the rich amine was between 0.51 and 0.67 moles per mole of MEA. A 15.3 weight percent solution of MEA was used.

Various ratios of $H_2S:CO_2$ in the sour gas feed were used; however for the contactor used the ppm $H_2S$ in the sweet gas was independent of this ratio at given $H_2S$ and

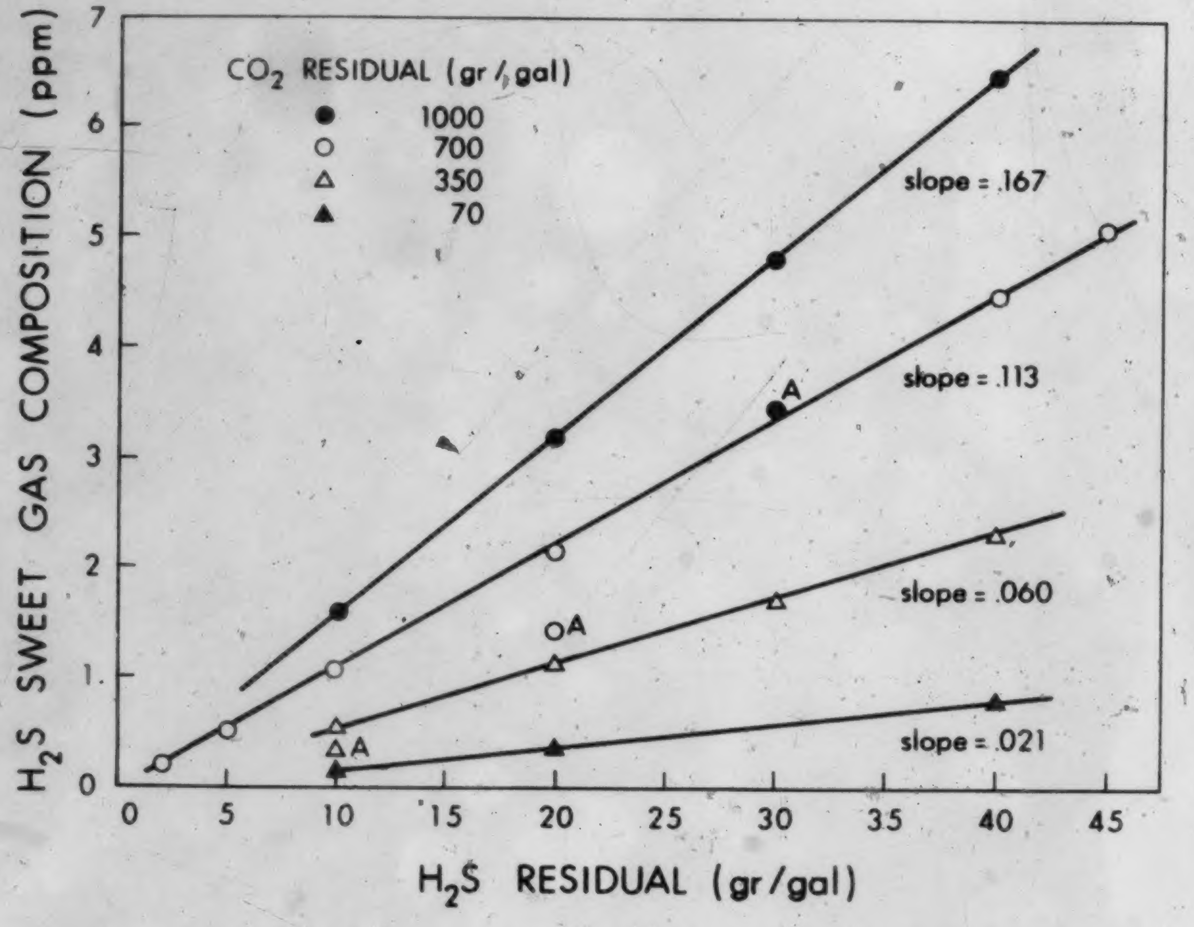


FIGURE 3: COMPOSITION OF $H_2S$ IN SWEET GAS VERSUS $H_2S$ LEAN AMINE RESIDUAL

$CO_2$ lean amine residuals. This is apparently because the number of ideal stages used is more than adequate in terms of producing an overheads specification on $H_2S$. Any dependence of the $H_2S$ sweet gas composition on the $H_2S:CO_2$ feed ratio could be determined by repeating the study with a column of fewer ideal stages (say 4 or less).

Four different $CO_2$ residual compositions were used. At a given value of $CO_2$ residual the amount of $H_2S$ in the sweet gas increases linearly with $H_2S$ residual. The presence of $CO_2$ affects the degree to which $H_2S$ may be absorbed. The slopes of the straight lines on Figure 3 increase approximately linearly with increasing $CO_2$ residual. Thus stripping of the $CO_2$ to a low level in the regenerator will facilitate $H_2S$ absorption in the contactor.

In the design of a sweetening system, a prime requirement is meeting the pipeline specifications on $H_2S$ in the sweet gas. Knowing this specification one can use a graph such as Figure 3 to select particular $H_2S$ and $CO_2$ residuals in the lean amine that will result in an acceptable level of $H_2S$ in the product. The regenerator must then be designed so as to strip the lean amine to the required degree. This amounts to a multivariable problem because the $H_2S$ and $CO_2$ residuals are not independent[30]. According to the plot of Fitzgerald and Richardson[9] the usual range of interest would be $CO_2$ residuals of 1000 -

grains per gallon or greater, for feed ratios less than 3 moles of $H_2S$ per mole of $CO_2$. This corresponds to the upper lines in Figure 3. For a reasonable stripper design, the same authors indicate that $H_2S$ would be stripped to a residual of less than 40 grains per gallon except in cases where the sour gas feed is predominantly $H_2S$.

The actual positioning of the points on Figure 3 depends on the equilibrium data correlation employed. To illustrate this, three of the runs were duplicated using the AMOCO correlation. The points are marked with an 'A', and it is seen that the predicted $H_2S$ compositions in the sweet gas are lower than those given by the other correlation. However, neither correlation can claim greater accuracy than the other as the region covered by Figure 3 lies outside the range of any hitherto published data. For both data correlations the predicted solubilities are therefore an extrapolation of trends in the region of higher $H_2S$ loadings. Experimental data in the region of very low $H_2S$ loadings, that is down to 0.01 moles/mole amine or lower, would allow a more accurate evaluation of the dependence of the sweet gas $H_2S$ composition on the lean amine residuals.

## 4.4 Prediction of Stage Efficiencies

The stage efficiencies for $H_2S$ and $CO_2$ are calculated from equation (2-11). Of the variables in this equation, the overall mass transfer coefficient, $K_{OG}a$, is the only one not trivially obtained from the current values of the stage variables. For $CO_2$ $K_{OG}a$ will be estimated directly from equation (2-14), which is a general correlation for bubble cap trays given by Kohl and Riesenfeld[24]. $K_{OG}a$ for $H_2S$ will be estimated from equation (2-12); thus estimates are required for $k_g a$, $k_L^o$, a and I. Values of the individual phase mass transfer coefficients and interfacial area per volume of plate are estimated via the following formulae given by Danckwerts[7] for bubble cap plates

$$k_G = 7\ u^{0.25}\ S^{-0.5}\ D_G^{\ 0.5} \qquad (4\text{-}1)$$

$$k_L^o = 11\ u^{0.25}\ S^{-0.5}\ D_A^{\ 0.5} \qquad (4\text{-}2)$$

$$a = 0.7\ u^{0.5}\ S^{0.833} \qquad (4\text{-}3)$$

where: $D_G$ is the diffusivity of $H_2S$ in the gas phase $cm^2/s$, and can be estimated as given in Treybal[43]

$D_A$ = diffusivity of $H_2S$ in the liquid phase ($cm^2/s$)

u = volumetric gas flow rate per unit area of plate (cm/s)

S = volume of liquid on plate per unit area of plate ($cm^3/cm^2$)

a" = interfacial area per unit area of plate ($cm^2/cm^2$)

$k_G$, $k_L^o$ have units of cm/s.

The column diameter can be estimated from charts given by Maddox[30], thus giving the cross-sectional area . The average depth of liquid on the plate, $z_T$, can be calculated using standard design techniques[43]. Knowing this enables S in equations (4-1) to (4-3) above to be calculated. Then the interfacial area per volume of plate is:

$$a = a''/z_T \tag{4-4}$$

Finally $k_Ga$ is given from $k_G$ by the equation

$$k_ga = \frac{k_Ga}{RT} \tag{4-5}$$

The enhancement factor I is estimated from equation (2-15).

### 4.4.1 $CO_2$ Stage Efficiency

The various terms in equation (2-14) are calculated as follows:

(i) Data on the viscosity of amine solutions[11] was approximately curvefitted by the equation:

$$\ell n\ \mu = 0.96 + 0.036(wt - 0.10) - 0.011T \tag{4-6}$$

where: $\mu$ is in cp

wt = weight fraction of amine

T = temperature (°F)

(ii) The values of $X_{CO_2}$, T and p are given by the current values of the stage variables.

(iii) $z_T$ is known from Section 4.4, and V can be calculated from the molar flowrate and cross-sectional area.

### 4.4.2 $H_2S$ Stage Efficiency

The bulk phase concentration of free amine can be calculated as follows. The concentration of amine at the top of the absorber is given by:

$$[RNH_2]_{top} = 1000\rho_L(z_3 - 2z_2 - z_1)/XM_{av} \quad (4\text{-}7)$$

where: $z_1$, $z_2$, $z_3$ are respectively the quantities of $H_2S$, $CO_2$ and MEA in the lean amine (mole/mole solution).

$XM_{av}$ is the average molecular weight of the lean amine (g/gmole).

$\rho_L$ is the density of the amine solution (g/cm$^3$), and is given approximately by equation (4-8).

$$\rho_L = 1.002 + .052(wt - .10) - .000278(T-68) + .001(6 - 20\,wt)(T-68)^{0.5} \quad (4\text{-}8)$$

where wt and T are the same as in equation (4-6).

The amount of $CO_2$ absorbed above plate j in the column is given by:

$$(CO_2)_{abs} = \frac{1000\rho_L}{XM_{av}}\left\{\frac{V_j}{L_j}\, y_{2,j} - \frac{V_1}{L_1}\, y_{2,1}\right\} \quad (4\text{-}9)$$

Similarly the quantity of $H_2S$ absorbed above plate j can be calculated. Then, as two moles of amine react with one mole of $CO_2$, the concentration of free amine in solution on plate j is:

$$[RNH_2]_j = [RNH_2]_{top} - 2 \cdot (CO_2)_{abs} - (H_2S)_{abs} \quad (4.10)$$

It is necessary to iterate to determine the value of $K_{OG}a$ because the interfacial partial pressure is unknown, yet the enhancement factor and hence $K_{OG}a$ depend on it. The iterative procedure is as follows:

(i) Assume the interfacial partial pressure, $p_{int}$.

(ii) Calculate I from equation (2-15). The solubilities $C'_{o,1}$ and $C'_{o,2}$ are obtained from a Henry's Law expression and the bulk phase concentration of amine is given by equation (4-10).

(iii) Calculate $K_{OG}a$ from equation (2-12).

(iv) Calculate the mean rate of absorption of $H_2S$ as

$$\overline{V}a = K_{OG}a \cdot p_{H_2S} \qquad (4\text{-}11)$$

(v) Calculate the actual interfacial partial pressure as

$$p_{int} = p_{H_2S} - \frac{\overline{V}a}{k_g a} \qquad (4\text{-}12)$$

(vi) Repeat steps (i) to (v) until a constant value of $\overline{V}a$ is achieved.

### 4.4.3 Example Problem No. 5

Example problem 1 was used, with 8 stages and the inclusion of the above methods to calculate vapourization efficiencies for $H_2S$ and $CO_2$. All other efficiencies were set equal to unity. The physical parameters required for the problem are as follows:

$$\text{Diffusivities} - \left.\begin{array}{ll} H_2S & 1.2 \\ CO_2 & 1.4 \\ \text{MEA} & 0.77 \end{array}\right\} \times 10^{-5}\ (\text{cm}^2/\text{s})$$

For $H_2S$ absorption - $k_L^o$ = .033 cm/s

$k_g a$ = $1.0 \times 10^{-6}$ gmole/cm$^3$.atm.s

a = 4.3 cm$^2$ interfacial area/cm$^3$ liquid

Column cross-sectional area = 6900 cm$^2$

Average depth of liquid on a stage = 13 cm.

The computer printout for the example is given in Appendix 4.9. The vapourization efficiencies display a definite trend down the column for both $CO_2$ and $H_2S$. They increase between the top stage and the stage on which the semilean amine is introduced, and then display the same trend between the semilean amine feed stage and the bottom.

The efficiencies are much greater than unity on a number of stages, and particularly so for $CO_2$. These numbers may be more familiarly represented by backing out the Murphree vapour efficiencies using the equation derived as follows. The Murphree efficiency is defined as:

$$E_{MVi,j} = \frac{y_{i,j} - y_{i,j+1}}{K_{i,j}\, x_{i,j} - y_{i,j+1}} \qquad (4\text{-}13)$$

Substituting for $K_{i,j}\, x_{i,j}$ from equation (3-1), that is, $K_{i,j}\, x_{i,j} = y_{i,j}/e_{i,j}$ (4-14)

and rearranging, yields

$$E_{MVi,j} = \frac{e_{i,j}\left(\dfrac{y_{i,j+1}}{y_{i,j}} - 1\right)}{\left(e_{i,j}\,\dfrac{y_{i,j+1}}{y_{i,j}}\right) - 1} \qquad (4\text{-}15)$$

Table 4 details the Murphree efficiencies for each stage in the column. The values show selective absorption of $H_2S$ over $CO_2$ below the semilean feed tray, and in magnitude the efficiencies agree with the rule of thumb values of 0.8 for $H_2S$ and 0.3 for $CO_2$. To illustrate the difference between calculating the efficiencies and using ideal stages, the same problem was run with 4 ideal stages, with

TABLE 4: MURPHREE EFFICIENCIES AS CALCULATED FROM VAPOURIZATION EFFICIENCIES

| Stage | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| $H_2S$ | 0.92 | 0.84 | 1.03 | 0.89 | 0.84 | 0.83 | 0.82 | 0.82 |
| $CO_2$ | 1.00 | 0.96 | 0.26 | 0.36 | 0.36 | 0.35 | 0.35 | 0.33 |

the semilean amine feeding to stage 3. In the 8-tray case the sweet gas contained 32 ppm $H_2S$, while 4 ideal trays reduced the $H_2S$ to only 14 ppm in the sweet gas. A further distinction between "real" and ideal stages is that absorption occurs over a larger number of trays in the former case than in the latter. This produces a more slowly variant vapour profile up the column for calculations incorporating vapourization efficiencies.

# 5. A GENERAL ALGORITHM FOR SOLVING MULTICOLUMN SYSTEMS.

## 5.1 Model Equations

A general network of columns may be considered a system of columns in which any stage may have, in addition to an external feed stream, one or more feed streams which originated at another stage in the network. Thus any stage in the general network is represented by Figure 4. There are four possible types of interconnected stream, namely a liquid side stream, vapour side stream, bottoms liquid product stream or top vapour product stream. For convenience in the following discussion, the bottom stage of a column in the system will be subscripted with the symbol NB, and the top stage with the symbol NT.

Equations (3-1), (3-3), (3-4), (3-5) and (3-6) represent the model equations for a single column. In a general network of columns, the material and energy balance equations for a stage must be modified to include the sum of the contributions from interconnected streams entering that stage. That is, equations (3-6), (3-3) and (3-5) for stage j and component i become as follows:

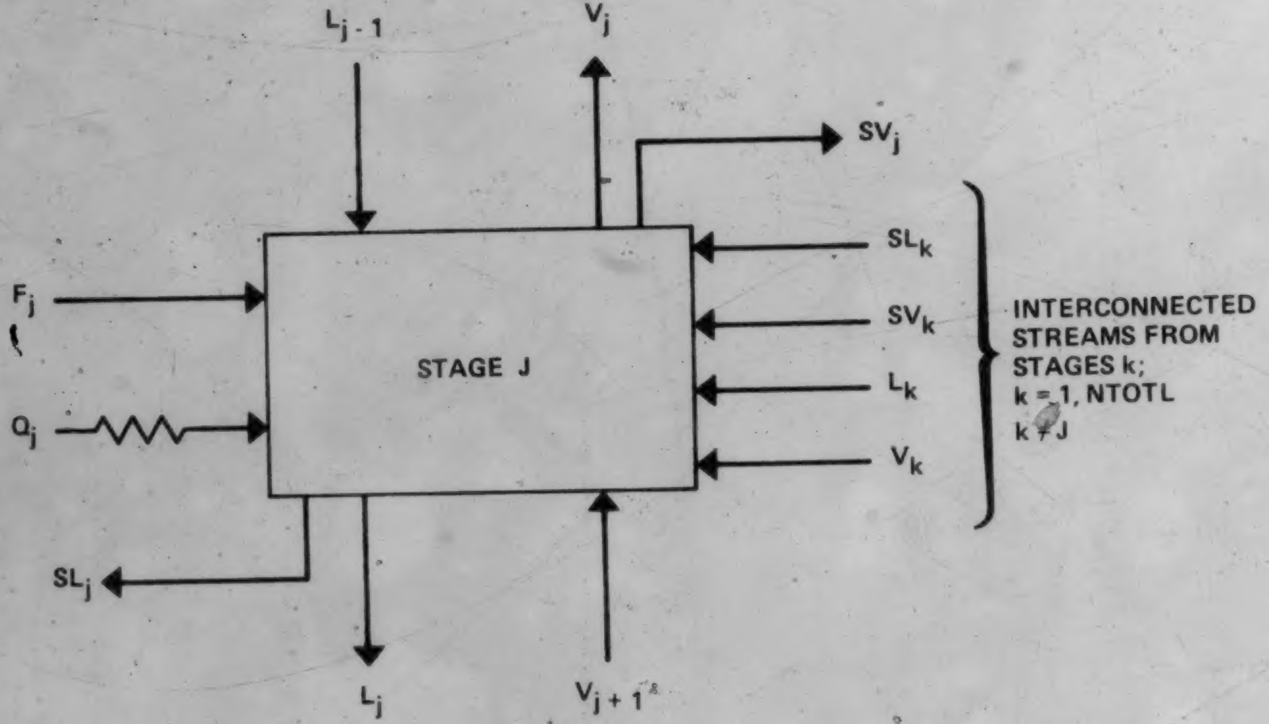

$L_{j-1}$
$V_j$
$SV_j$
$F_j$
$Q_j$
STAGE J
$SL_k$
$SV_k$
$L_k$
$V_k$
INTERCONNECTED STREAMS FROM STAGES k;
k = 1, NTOTL
k ≠ J
$SL_j$
$L_j$
$V_{j+1}$

FIGURE 4: GENERAL STAGE IN A MULTICOLUMN SYSTEM

## Component Material Balance

$$F_j z_{i,j} + L_{j-1} x_{i,j-1} + V_{j+1} e_{i,j+1} K_{i,j+1} x_{i,j+1}$$

$$- (L_j + SL_j)x_{i,j} - (V_j + SV_j)e_{i,j} K_{i,j} x_{i,j}$$

$$+ \sum_k \psi_{c,i,k} \equiv c_{i,j} \tag{5-1}$$

$1 \leqslant i \leqslant NCP, \quad 1 \leqslant j \leqslant NTOTL$

## Energy Balance

$$F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} - (L_j + SL_j)h_j$$

$$- (V_j + SV_j)H_j + \sum_k \psi_{E,k} \equiv E_j \tag{5-2}$$

$1 \leqslant j \leqslant NTOTL$

## Overall Material Balance

$$F_j + L_{j-1} + V_{j+1} - (L_j + SL_j) - (V_j + SV_j)$$

$$+ \sum_k \psi_{M,k} \equiv M_j \tag{5-3}$$

$1 \leqslant j \leqslant NTOTL$

where for the various types of interconnected stream, $\psi_{c,i,k}$, $\psi_{E,k}$ and $\psi_{M,k}$ are as given in Table 5, with k denoting the leaving stage of a particular stream. The phase relation and summation equations remain the same as (3-1) and (3-4).

TABLE 5: CONTRIBUTION OF INTERLINKED STREAMS TO MATERIAL AND ENERGY BALANCE EQUATIONS.

| Type of Stream | $\psi_{c,i,k}$ | $\psi_{E,k}$ | $\psi_{M,k}$ |
|---|---|---|---|
| Liquid side stream | $SL_k\ x_{i,k}$ | $SL_k\ h_k$ | $SL_k$ |
| Vapour side stream | $SV_k\ e_{i,k}\ K_{i,k}\ x_{i,k}$ | $SV_k\ H_k$ | $SV_k$ |
| Liquid product | $L_k\ x_{i,k}$ | $L_k\ h_k$ | $L_k$ |
| Vapour product | $V_k\ e_{i,k}\ K_{i,k}\ x_{i,k}$ | $V_k\ H_k$ | $V_k$ |

The summation in equations (5-1) to (5-3) indicates the possibility of more than one interconnected stream entering stage j.

## 5.2 Linearized Equations

The equations are written for each stage in the interconnected system of columns, and then linearized using the same procedure as for individual columns. The linearized equations are:

## Component Material Balance

$$
\begin{aligned}
& L_{j-1}\,\Delta x_{i,j-1} - \left[(L_j+SL_j)+(V_j+SV_j)e_{i,j}\left(K_{i,j}+x_{i,j}\frac{\partial K_{i,j}}{\partial x_{i,j}}\right)\right]\Delta x_{i,j} \\
& + V_{j+1}\,e_{i,j+1}\left(K_{i,j+1}+x_{i,j+1}\frac{\partial K_{i,j+1}}{\partial x_{i,j+1}}\right)\Delta x_{i,j+1} \\
& + \sum_k \eta_{c,i,k}\,\Delta x_{i,k} - (V_j+SV_j)e_{i,j}\,x_{i,j}\frac{\partial K_{i,j}}{\partial T_j}\Delta T_j \\
& + V_{j+1}\,e_{i,j+1}\,x_{i,j+1}\frac{\partial K_{i,j+1}}{\partial T_{i,j+1}}\Delta T_{j+1} + \sum_k \mu_{c,k}\,\Delta T_k \\
& + x_{i,j-1}\,\Delta L_{j-1} - x_{i,j}\,\Delta L_j - y_{i,j}\,\Delta V_j \\
& + y_{i,j+1}\,\Delta V_{j+1} + \sum_k \tau_{c,k} = -c_{i,j} \qquad (5\text{-}4)
\end{aligned}
$$

At $J = NT$

$$
\begin{aligned}
& -[(L_{NT}+SL_{NT}) + V_{NT}\,e_{i,NT}\left(K_{i,NT}+x_{i,NT}\frac{\partial K_{i,NT}}{\partial x_{i,NT}}\right)]\,\Delta x_{i,NT} \\
& + V_{NT+1}\,e_{i,NT+1}\left(K_{i,NT+1}+x_{i,NT+1}\frac{\partial K_{i,NT+1}}{\partial x_{i,NT+1}}\right)\Delta x_{i,NT+1} \\
& + \sum_k \eta_{c,i,k}\,\Delta x_{i,k} - V_{NT}\,e_{i,NT}\,x_{i,NT}\frac{\partial K_{i,NT}}{\partial T_{NT}}\Delta T_{NT} \\
& + V_{NT+1}\,e_{i,NT+1}\,x_{i,NT+1}\frac{\partial K_{i,NT+1}}{\partial T_{i,NT+1}}\Delta T_{NT+1} \\
& + \sum_k \mu_{c,k}\,\Delta T_k - x_{i,NT}\,\Delta L_{NT} - y_{i,NT}\,\Delta V_{NT} + y_{i,NT+1}\,\Delta V_{NT+1} \\
& + \sum_k \tau_{c,k} = -c_{i,NT} \qquad (5\text{-}4\text{-}a)
\end{aligned}
$$

At J = NB

$$L_{NB-1}\Delta x_{i,NB-1} - [L_{NB} + (V_{NB}+SV_{NB}) e_{i,NB} (K_{i,NB} + x_{i,NB} \frac{\partial K_{i,NB}}{\partial x_{i,NB}})] \Delta x_{i,NB}$$

$$+ \sum_k \eta_{c,i,k} \Delta x_{i,k}$$

$$- (V_{NB} + SV_{NB}) e_{i,NB}\, x_{i,NB} \frac{\partial K_{i,NB}}{\partial T_{NB}} \Delta T_{NB}$$

$$+ \sum_k \mu_{c,k} \Delta T_k + x_{i,NB-1} \Delta L_{NB-1} - x_{i,NB} \Delta L_{NB} - y_{i,NB} \Delta V_{NB}$$

$$+ \sum_k \tau_{c,k} = - c_{i,NB} \qquad (5\text{-}4\text{-}b)$$

Energy Balance

$$L_{j-1} \frac{\partial h_{j-1}}{\partial T_{j-1}} \Delta T_{j-1} - [(L_j+SL_j) \frac{\partial h_j}{\partial T_j} + (V_j+SV_j) \frac{\partial H_j}{\partial T_j}] \Delta T_j$$

$$+ V_{j+1} \frac{\partial H_{j+1}}{\partial T_{j+1}} \Delta T_{j+1} + \sum_k \mu_{E,k} \Delta T_k + h_{j-1} \Delta L_{j-1}$$

$$- h_j \Delta L_j - H_j \Delta V_j + H_{j+1} \Delta V_{j+1} + \sum_k \tau_{E,k} = -E_j$$

$$(5\text{-}5)$$

At J = NT

$$- [(L_{NT} + SL_{NT}) \frac{\partial h_{NT}}{\partial T_{NT}} + V_{NT} \frac{\partial H_{NT}}{\partial T_{NT}}] \Delta T_{NT}$$

$$+ V_{NT+1} \frac{\partial H_{NT+1}}{\partial T_{NT+1}} \Delta T_{NT+1} + \sum_k \mu_{E,k} \Delta T_k - h_{NT} \Delta L_{NT} - H_{NT} \Delta V_{NT}$$

$$+ H_{NT+1} \Delta V_{NT+1} + \sum_k \tau_{E,k} + \Delta Q_{NT} = - E_{NT} \qquad (5\text{-}5\text{-}a)$$

where $\Delta Q_{NT} = 0$ for an absorber or reboiled absorber.

At J = NB

$$L_{NB-1} \frac{\partial h_{NB-1}}{\partial T_{NB-1}} \Delta T_{NB-1} - [L_{NB} \frac{\partial h_{NB}}{\partial T_{NB}} + (V_{NB}+SV_{NB}) \frac{\partial H_{NB}}{\partial T_{NB}}] \Delta T_{NB}$$

$$+\sum_k \mu_{E,k} \Delta T_k + h_{NB-1} \Delta L_{NB-1} - h_{NB} \Delta L_{NB} - H_{NB} \Delta V_{NB} + \sum_k \tau_{E,k}$$

$$+ \Delta Q_{NB} = - E_{NB} \qquad (5\text{-}5\text{-}b)$$

where $\Delta Q_{NB} = 0$ for an absorber.

Overall Material Balance

$$\Delta L_{j-1} - \Delta L_j - \Delta V_j + \Delta V_{j+1} + \sum_k \tau_{M,k} = - M_j \qquad (5\text{-}6)$$

At J = NT

$$- \Delta L_{NT} - \Delta V_{NT} + \Delta V_{NT+1} + \sum_k \tau_{M,k} = - M_{NT} \qquad (5\text{-}6\text{-}a)$$

At J = NB

$$\Delta L_{NB-1} - \Delta L_{NB} - \Delta V_{NB} + \sum_k \tau_{M,k} = - M_{NB} \qquad (5\text{-}6\text{-}b)$$

The terms in $\eta$, $\mu$ and $\tau$ in equations (5-4) to (5-6) arise from the presence of interconnected streams. For example, the terms $\psi_{c,i,k}$ in equation (5-1) give rise to the terms $\eta_{c,i,k}$, $\mu_{c,k}$ and $\tau_{c,k}$ in equation (5-4).

## TABLE 6: TERMS IN LINEARIZED EQUATIONS ARISING FROM INTERCONNECTED STREAMS

| Type of Stream | $\eta_{c,i,k}$ | $\mu_{c,k}$ | $\tau_{c,k}$ | $\mu_{E,k}$ | $\tau_{E,k}$ | $\tau_{M,k}$ |
|---|---|---|---|---|---|---|
| Liquid side stream | $SL_k$ | 0 | 0 | $SL_k \frac{\partial h_k}{\partial T_k}$ | 0 | 0 |
| Vapour side stream | $SV_k\ e_{i,k}(K_{i,k}+x_{i,k}\frac{\partial K_{i,k}}{\partial x_{i,k}})$ | $SV_k\ e_{i,k}\ x_{i,k}\frac{\partial K_{i,k}}{\partial T_k}$ | 0 | $SV_k \frac{\partial H_k}{\partial T_k}$ | 0 | 0 |
| Liquid product | $L_k$ | 0 | $x_{i,k}\ \Delta L_k$ | $L_k \frac{\partial h_k}{\partial T_k}$ | $h_k\ \Delta L_k$ | $\Delta L_k$ |
| Vapour product | $V_k\ e_{i,k}(K_{i,k}+x_{i,k}\frac{\partial K_{i,k}}{\partial x_{i,k}})$ | $V_k\ e_{i,k}\ x_{i,k}\frac{\partial K_{i,k}}{\partial T_k}$ | $y_{i,k}\ \Delta V_k$ | $V_k \frac{\partial H_k}{\partial T_k}$ | $H_k\ \Delta V_k$ | $\Delta V_k$ |

A summary of the values of $\eta_{c,i,k}$, $\mu_{c,k}$, $\tau_{c,k}$, $\mu_{E,k}$, $\tau_{E,k}$ and $\tau_{M,k}$ for each possible type of interconnected stream is given in Table 6.

## 5.3 Matrix Forms

In the model for single columns, the matrix form of the linearized equations contains a number of tridiagonal matrices. In particular, the coefficient matrices of $\overline{\Delta x_i}$ (liquid composition corrections) in the component material balance equations and of $\overline{\Delta T}$ (temperature corrections) in the energy balance are tridiagonal. The ease of inversion of these matrices facilitates the formulation of a solution.

The linearized equations for a multicolumn system (equations (5-4) to (5-6)) may also be represented in matrix form as follows:

$$\overline{A_i}\ \overline{\Delta x_i} + \overline{B_i}\ \overline{\Delta T} + \overline{D_i}\ \overline{\Delta V} + \overline{F_i}\ \overline{\Delta L} = \overline{C_i}$$

$$1 \leq i \leq NCP \tag{5-7}$$

$$\overline{P}\ \overline{\Delta T} + \overline{Q}\ \overline{\Delta V} + \overline{R}\ \overline{\Delta L} = \overline{E} \tag{5-8}$$

$$\overline{G}\ \overline{\Delta V} + \overline{H}\ \overline{\Delta L} = \overline{M} \tag{5-9}$$

However, in this case the presence of interconnected streams introduces off-tridiagonal elements into the matrices, in particular the coefficient matrices discussed above. Thus a non-trivial extension of the algorithm used to solve single column systems is required.

The detailed form of the matrices is more clearly understood by considering a particular network of columns, say that shown in Figure 5. The example system consists of three columns, each having 20 stages. There are four interconnected streams:

(1) a vapour product stream from the top stage of column I to stage 5 of column II

(2) a bottoms liquid product stream from stage 20 of column I to stage 1 of column III

(3) a liquid side stream from stage 14 of column II to stage 9 of column III

(4) a vapour side stream from stage 3 of column III to stage 12 of column I.

In general each coefficient matrix in equations (5-7), (5-8) and (5-9) has the form of the matrix shown in Figure 6. The matrix is basically block tridiagonal, with one diagonal block per separation device. Let the devices in the system be labelled I, II and III, and label the blocks in Figure 6 in the same fashion as elements of a matrix. Then off-tridiagonal elements, arising from the interconnected streams, appear as follows.

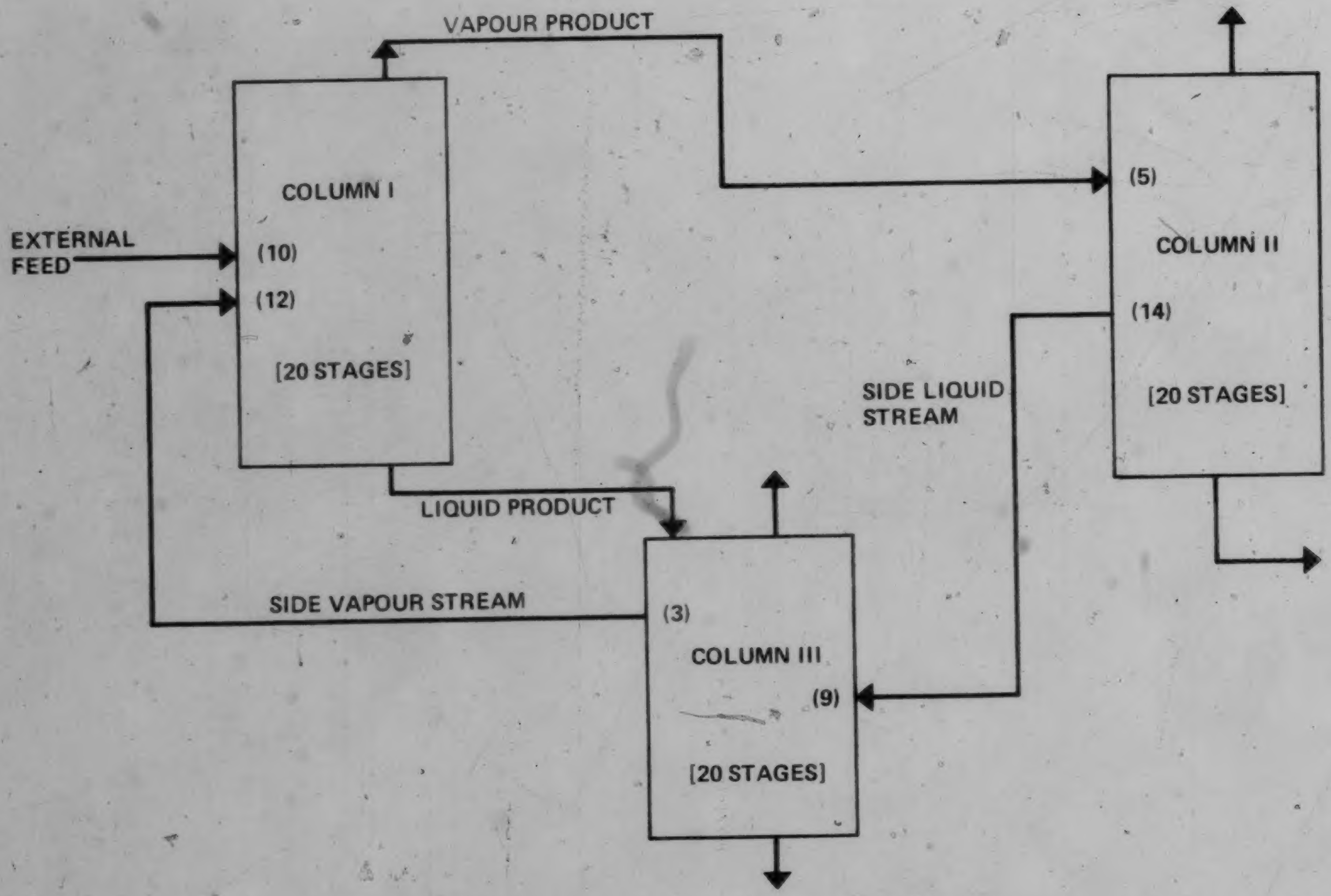

VAPOUR PRODUCT
COLUMN I
EXTERNAL FEED
(10)
(12)
[20 STAGES]
COLUMN II
(5)
(14)
[20 STAGES]
SIDE LIQUID STREAM
LIQUID PRODUCT
SIDE VAPOUR STREAM
(3)
COLUMN III
(9)
[20 STAGES]

FIGURE 5: EXAMPLE SYSTEM OF COLUMNS

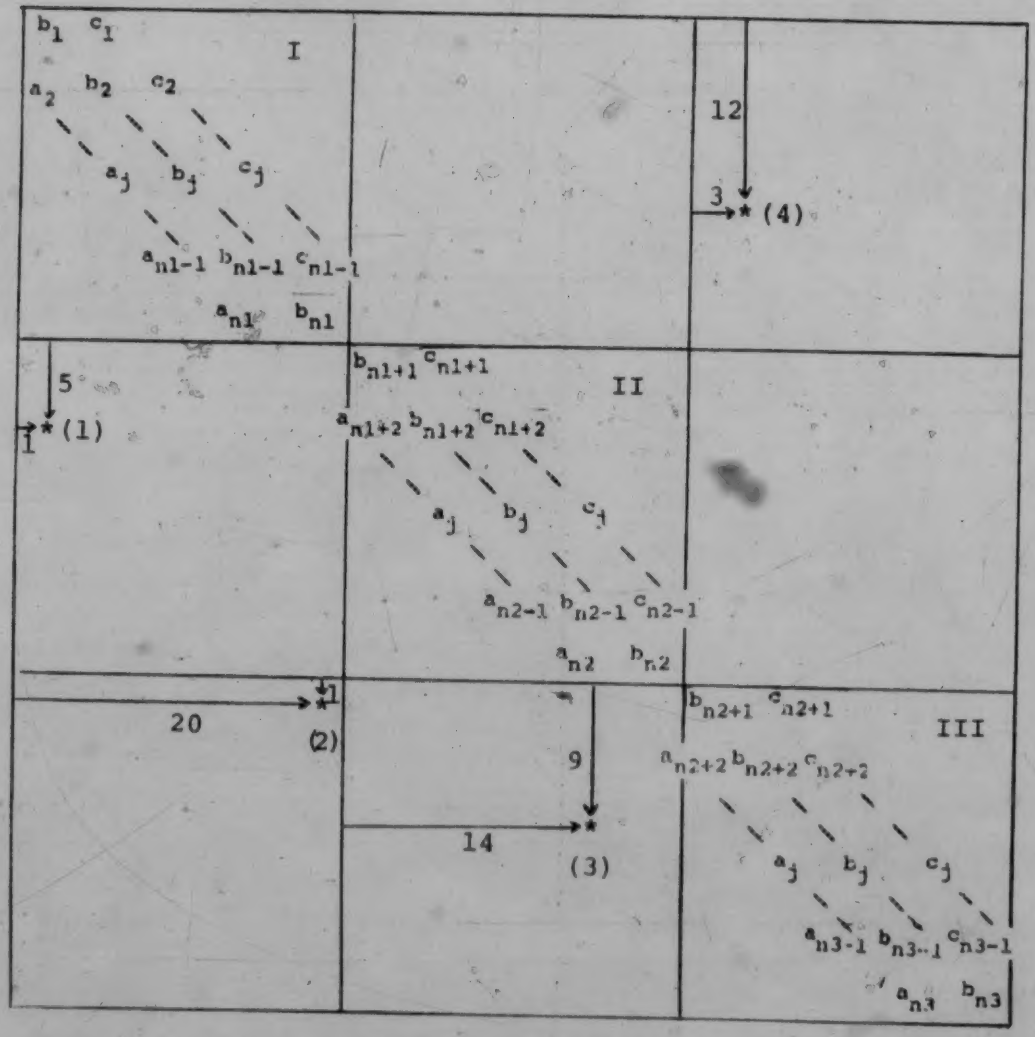

b1 c1
I
a2 b2 c2
aj bj cj
an1-1 bn1-1 cn1-1
an1 bn1
12
3
* (4)
5
1
* (1)
bn1+1 cn1+1
II
an1+2 bn1+2 cn1+2
aj bj cj
an2-1 bn2-1 cn2-1
an2 bn2
1
20
* (2)
9
14
* (3)
bn2+1 cn2+1
III
an2+2 bn2+2 cn2+2
aj bj cj
an3-1 bn3-1 cn3-1
an3 bn3

FIGURE 6: GENERAL MATRIX FORM

If an interconnected stream goes from device III to device I, the appropriate off-tridiagonal element appears in block (I,III). The exact position of the element is given by the entering and leaving stages. For example, for stream (4) above it is at position (12,3) inside block (I,III). Other off-tridiagonal elements may occupy the positions indicated on Figure 6. A given off-tridiagonal position in the matrix will represent a unique interconnected stream. Also note that theoretically an off-tridiagonal element could appear in one of the diagonal blocks. This would correspond to a connected stream going between different stages of the same device and is not likely to occur in practice.

Depending on the type of interconnected stream, some off-tridiagonal elements in the coefficient matrices may be zero (see Table 6). For interconnected streams (1) to (4) given above, Table 7 lists which streams will contribute a non-zero element. The value of these non-zero elements can be read off Table 6.

## TABLE 7: NON-ZERO OFF-TRIDIAGONAL ELEMENTS IN EACH COEFFICIENT MATRIX

| Equation | Coefficient of: | | | |
|---|---|---|---|---|
| | $\overline{\Delta x_i}$ | $\overline{\Delta T}$ | $\overline{\Delta V}$ | $\overline{\Delta L}$ |
| component material balance | 1,2,3,4 | 1,4 | 1 | 2 |
| energy balance | na | 1,2,3,4 | 1 | 2 |
| overall material balance | na | na | 1 | 2 |

na ≡ not applicable

In each diagonal block the elements $a_j$, $b_j$ and $c_j$ will be the same as for a single separation device. Thus, these elements are as follows for the various coefficient matrices in equations (5-7), (5-8) and (5-9).

(1) Matrix $\overline{A_i}$

$$a_{NT} = 0$$

$$b_{NT} = -(L_{NT} + SL_{NT}) - V_{NT}\, e_{i,NT}\left(K_{i,NT} + x_{i,NT} \frac{\partial K_{i,NT}}{\partial x_{i,NT}}\right)$$

$$c_{NT} = V_{NT+1}\, e_{i,NT+1}\left(K_{i,NT+1} + x_{i,NT+1} \frac{\partial K_{i,NT+1}}{\partial x_{i,NT+1}}\right)$$

$$a_j = L_{j-1}$$

$$b_j = -(L_j + SL_j) - (V_j + SV_j) e_{i,j} \left(K_{i,j} + x_{i,j} \frac{\partial K_{i,j}}{\partial x_{i,j}}\right)$$

$$c_j = V_{j+1}\, e_{i,j+1} \left(K_{i,j+1} + x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial x_{i,j+1}}\right)$$

$j = NT+1 \rightarrow NB-1$

$$a_{NB} = L_{NB-1}$$

$$b_{NB} = -\,L_{NB} - (V_{NB} + SV_{NB}) e_{i,NB} \left(K_{i,NB} + x_{i,NB} \frac{\partial K_{i,NB}}{\partial x_{i,NB}}\right)$$

$$C_{NB} = 0$$

(2) Matrix $B_i$

$$a_{NT} = 0$$

$$b_{NT} = -\,V_{NT}\, e_{i,NT}\, x_{i,NT} \frac{\partial K_{i,NT}}{\partial T_{NT}}$$

$$c_{NT} = V_{NT+1}\, e_{i,NT+1}\, x_{i,NT+1} \frac{\partial K_{i,NT+1}}{\partial T_{NT+1}}$$

$$a_j = 0$$

$$b_j = -\,(V_j + SV_j)\, e_{i,j}\, x_{i,j} \frac{\partial K_{i,j}}{\partial T_j}$$

$$c_j = V_{j+1}\, e_{i,j+1}\, x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial T_{j+1}}$$

$j = NT+1 \rightarrow NB-1$

$a_{NB} = 0$

$b_{NB} = -(V_{NB} + SV_{NB})\, e_{i,NB}\, x_{i,NB} \frac{\partial K_{i,NB}}{\partial T_{NB}}$

$c_{NB} = 0$

(3) Matrix $\overline{D_i}$

$a_j = 0$

$b_j = -y_{i,j}$

$c_j = y_{i,j+1}$ $\qquad j = NT \rightarrow NB-1$

$a_{NB} = 0$

$b_{NB} = -y_{i,NB}$

$c_{NB} = 0$

(4) Matrix $\overline{F_i}$

$a_{NT} = 0$

$b_{NT} = -x_{i,NT}$

$c_{NT} = 0$

$$a_j = x_{i,j-1}$$

$$b_j = -x_{i,j}$$

$$c_j = 0$$

$$j = NT+1 \rightarrow NB$$

(5) Matrix $\overline{P}$

$$a_{NT} = 0$$

$$b_{NT} = -[(L_{NT} + SL_{NT}) \frac{\partial h_{NT}}{\partial T_{NT}} + V_{NT} \frac{\partial H_{NT}}{\partial T_{NT}}]$$

$$c_{NT} = V_{NT+1} \frac{\partial H_{NT+1}}{\partial T_{NT+1}}$$

$$a_j = L_{j-1} \frac{\partial h_{j-1}}{\partial T_{j-1}}$$

$$b_j = -[(L_j + SL_j) \frac{\partial h_j}{\partial T_j} + (V_j + SV_j) \frac{\partial H_j}{\partial T_j}]$$

$$c_j = V_{j+1} \frac{\partial H_{j+1}}{\partial T_{j+1}}$$

$$j = NT+1 \rightarrow NB-1$$

$$a_{NB} = L_{NB-1} \frac{\partial h_{NB-1}}{\partial T_{NB-1}}$$

$$b_{NB} = -[L_{NB} \frac{\partial h_{NB}}{\partial T_{NB}} + (V_{NB} + SV_{NB}) \frac{\partial H_{NB}}{\partial T_{NB}}]$$

$$c_{NB} = 0$$

(6) Matrix $\overline{Q}$

$a_j = 0$

$b_j = - H_j$

$c_j = H_{j+1}$

$j = NT \rightarrow NB-1$

$a_{NB} = 0$

$b_{NB} = - H_{NB}$

$c_{NB} = 0$

(7) Matrix $\overline{R}$

$a_{NT} = 0$

$b_{NT} = - h_{NT}$

$c_{NT} = 0$

$a_j = h_{j-1}$

$b_j = - h_j$

$c_j = 0$

$j = NT+1 \rightarrow NB$

(8) Matrix $\overline{G}$

$a_j = 0$

$b_j = -1$

$c_j = +1$ $\qquad j = NT \rightarrow NB-1$

$a_{NB} = 0$

$b_{NB} = -1$

$c_{NB} = 0$

(9) Matrix $\overline{H}$

$a_{NT} = 0$

$b_{NT} = -1$

$c_{NT} = 0$

$a_j = +1$

$b_j = -1$

$c_j = 0$ $\qquad j = NT+1 \rightarrow NB$

### 5.4 Effect of Problem Specifications on Matrix Elements

For a specified column with a specified feed, the number of specifications is equal to the number of controllable variables. For a distillation column with a partial condenser these controllable variables are the reboiler and condenser duties, while for a reboiled absorber the reboiler duty is controllable. Thus two variables may be specified for a distillation column, and one for a reboiled absorber.

In the method presented by Harclerode and Gentry[14], the calculational procedure is limited to cases involving symmetrical specifications, where a symmetrical specification is one which applies to the same stage as the equation it replaces. For example, if the top vapour product is specified instead of the condenser duty, the specification is symmetrical.

With the current algorithm the limitation on specifications is not entirely the symmetrical consideration. Certain symmetrical specifications cannot be handled because the matrix $\bar{H}$ in equation (5-9) becomes singular. However, one other symmetrical specification, namely that of the bottoms liquid product in a reboiled absorber, also does not work even though no matrices are singular. The reason for this is unclear at present.

The following choices of specification have been successfully incorporated into the algorithm.

(a) Specification of the reflux ratio and quantity of reboiler vapour for a distillation column.

For the case of a partial condenser, $V_{NT+1}$ and $V_{NT}$ are related by the equation

$$V_{NT+1} = (1 + R)\, V_{NT} \tag{5-10}$$

As R is fixed it follows that

$$\Delta V_{NT} = \Delta V_{NT+1}/(1 + R) \tag{5-11}$$

Equation (5-11) is used to eliminate $\Delta V_{NT}$ from equations (5-4-a), (5-5-a) and (5-6-a). In the energy balance equation $\Delta Q_{NT}$ is non-zero, and this is placed into the position in the $\overline{\Delta V}$ matrix left vacant by the effective removal of $\Delta V_{NT}$ (by equation (5-11)). The reboiler vapour is fixed, giving $\Delta V_{NB} = 0$ in equations (5-4-b), (5-5-b) and (5-6-b). Similarly to the above, $\Delta Q_{NB}$ occupies the position of $\Delta V_{NB}$.

Correspondingly the following matrix elements are altered:

$$\text{in } \overline{D}_i, \quad b_{NT} = b_{NB} = C_{NB-1} = 0$$

$$c_{NT} = y_{i,NT+1} - \frac{y_{i,NT}}{(1+R)}$$

$$\text{in } \overline{Q}\ ,\quad b_{NT} = b_{NB} = 1.0$$

$$c_{NT} = H_{NT+1} - \frac{H_{NT}}{(1+R)}$$

$$c_{NB-1} = 0$$

$$\text{in } \overline{G}\ ,\quad b_{NT} = b_{NB} = c_{NB-1} = 0$$

$$c_{NT} = \frac{R}{(1+R)}$$

(b) An alternative specification for a distillation column is of condenser temperature and reboiler duty. In this case $\Delta T_{NT} = 0$ in equations (5-4-a) and (5-5-a) and $\Delta Q_{NT}$ occupies the position left vacant by $\Delta T_{NT}$. The following changes occur in the matrix elements:

$$\text{in } \overline{B_i},\quad b_{NT} = 0$$

$$\text{in } \overline{P}\ ,\quad b_{NT} = 1.0$$

$$a_{NT+1} = 0$$

(c) For a reboiled absorber the amount of reboiler vapour may be specified. Then $\Delta V_{NB} = 0$ and its position is occupied by $\Delta Q_{NB}$. Changes in the matrix elements are:

$$\text{in } \overline{D_i},\quad b_{NB} = c_{NB-1} = 0$$

$$\text{in } \overline{Q}\ ,\quad b_{NB} = 1.0$$

$$c_{NB-1} = 0$$

in $\overline{G}$ , $b_{NB} = c_{NB-1} = 0$

(d) For a reboiled absorber with reboiler duty specified, or for a distillation column with reboiler and condenser duties specified, no changes are necessary to the matrix elements.

## 5.5 Solution Procedure

The linearized equations (5-4, 5-5 and 5-6) may be expressed in matrix form as:

$$\overline{A_i}\ \overline{\Delta x_i} + \overline{B_i}\ \overline{\Delta T} + \overline{D_i}\ \overline{\Delta V} + \overline{F_i}\ \overline{\Delta L} = \overline{C_i} \qquad (5\text{-}7)$$

$$1 \leqslant i \leqslant NCP$$

$$\overline{P}\ \overline{\Delta T} + \overline{Q}\ \overline{\Delta V} + \overline{R}\ \overline{\Delta L} = \overline{E} \qquad (5\text{-}8)$$

$$\overline{G}\ \overline{\Delta V} + \overline{H}\ \overline{\Delta L} = \overline{M} \qquad (5\text{-}9)$$

In the case of a single column, equation (5-9) can be solved algebraically for the $\Delta L_j$ in terms of the $\Delta V_j$'s. The presence of interconnected streams (i.e. off-tridiagonal elements) precludes this possibility and equation (5-9) must be solved using matrix methods. This is readily done, by setting $\overline{M}$ equal to the zero matrix.

Assuming a solution to (5-9) has been obtained so that one may write:

$$\overline{\Delta L} = \overline{G^T}\ \overline{\Delta V} \tag{5-12}$$

then substitution of equation (5-12) into equations (5-7) and (5-8) reduces them to the form of equations (5-13) and (5-14)

$$\overline{A_i}\ \overline{\Delta x_i} + \overline{B_i}\ \overline{\Delta T} + \overline{D_i}\ \overline{\Delta V} = \overline{C_i}, \tag{5-13}$$

$$1 \leq i \leq NCP$$

$$\overline{P}\ \overline{\Delta T} + \overline{Q}\ \overline{\Delta V} = \overline{E} \tag{5-14}$$

These equations are identical in form to those for a single column; however, each matrix may include off-tridiagonal elements. In particular, $\overline{A_i}$ has the same number of off-tridiagonal elements as there are connected streams (see section 5.3). The rapidity of the solution procedure relies on easy conversion of $\overline{A_i}$ to a unit matrix, hence its pseudo-tridiagonal character is crucial.

Denote $\overline{A_i}$ as the sum of two matrices:

$$\overline{A_i} = \overline{A_{T,i}} + \overline{A_{OD,i}} \tag{5-15}$$

where: $\overline{A_{T,i}}$ is strictly tridiagonal

$\overline{A_{OD,i}}$ is a sparse matrix containing all zeros except for the off-tridiagonal elements in $\overline{A_i}$.

The method of solution of (5-13) and (5-14) is then as follows:

(i) Invert $\overline{A_{T,i}}$ using a suitable algebraic algorithm for tridiagonal matrices. Examples are the Thomas algorithm or the modification derived by Ishii[17].

(ii) Multiply equation (5-13) by the inverse of $\overline{A_{T,i}}$. Using (5-15) this produces:

$$\{\overline{I} + (\overline{A_{T,i}})^{-1}\,\overline{A_{OD,i}}\}\,\overline{\Delta x_i} + \overline{B_i}'\,\overline{\Delta T} + \overline{D_i}'\,\overline{\Delta V} = \overline{C_i}' \qquad (5\text{-}16)$$

The matrix $(\overline{A_{T,i}})^{-1}\,\overline{A_{OD,i}}$ consists of as many non-zero columns as there are interconnected streams entering different stages; all other columns consisting solely of zeros. Therefore:

(iii) Eliminate each non-zero column in turn by row-wise elimination on the matrix $\{\overline{I} + (\overline{A_{T,i}})^{-1}(\overline{A_{OD,i}})\}$, pivoting around the diagonal element and applying the procedure to all terms in equation (5-16), thus reducing it to the form

$$\overline{I}\,\overline{\Delta x_i} + \overline{B_i}\,\overline{\Delta T} + \overline{D_i}\,\overline{\Delta V} = \overline{C_i} \qquad (5\text{-}17)$$

(iv) Sum equation (5-17) over each component to yield:

$$\overline{I}\,\Sigma\,\overline{\Delta x_i} + \overline{B}\,\overline{\Delta T} + \overline{D}\,\overline{\Delta V} = \overline{C} \qquad (5\text{-}18)$$

Then using equation (3-10) with $S_j = 0$ reduces equation (5-18) to an equation of the form:

$$\overline{B}\ \overline{\Delta T} + \overline{D}\ \overline{\Delta V} = \overline{C} \qquad (5\text{-}19)$$

(v) Apply the procedure of steps (i) to (iii) to equation (5-14), reducing it to the form

$$\overline{I}\ \overline{\Delta T} + \overline{Q}\ \overline{\Delta V} = \overline{E} \qquad (5\text{-}20)$$

(vi) Equations (5-19) and (5-20) are then solved simultaneously to yield $\overline{\Delta T}$ and $\overline{\Delta V}$; $\overline{\Delta L}$ is obtained from equation (5-12).

(vii) These values are substituted back into equation (5-7) for each i, and the equation solved for the $\Delta x_{i,j}$. This again involves the manipulations of steps (i) to (iii).

(viii) New values of the temperature, vapour, liquid and composition profiles are calculated as follows, where t is an appropriate weighting factor ($0 < t \leq 1$)

$$T_j^{k+1} = T_j^{k} + t\ \Delta T_j \qquad (5\text{-}21)$$

$$V_j^{k+1} = V_j^{k} + t\ \Delta V_j \qquad (5\text{-}22)$$

$$x_{i,j}^{k+1} = x_{i,j}^{k} + t\ \Delta x_{i,j} \qquad (5\text{-}23)$$

$$y_{i,j} = K_{i,j}\ x_{i,j} \qquad (5\text{-}24)$$

and the new $L_j$'s are evaluated from the overall material balance equation (5-3) with $M_j = 0$. This avoids truncation errors associated with computing the new $L_j$'s from the old values and the corrections $\overline{\Delta L}$.

(ix) The $x_{i,j}$'s are normalized to avoid truncation error, and then $K_{i,j}$, $H_j$, $h_j$, $\frac{\partial K_{i,j}}{\partial T_j}$, $\frac{\partial K_{i,j}}{\partial x_{i,j}}$, $\frac{\partial H_j}{\partial T_j}$ and $\frac{\partial h_j}{\partial T_j}$ calculated.

The elements of the matrices are obtained using these values and the updated values of the stage variables.

(x) Calculations are continued until the following convergence criterion is satisfied:

$$\frac{[\mathrm{CRIT}]}{\mathrm{NTOTL}} \leq \text{tolerance} = 10^{-6} \qquad (5\text{-}25)$$

where [CRIT] is defined as

$$[\mathrm{CRIT}] = \sum_{j=1}^{\mathrm{NTOTL}} \left[ \left( \sum_{i=1}^{\mathrm{NCP}} y_{i,j} - 1.0 \right)^2 + \left\{ E_j / \left( F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} + \sum_k \psi_{E,k} \right) \right\}^2 \right] \qquad (5\text{-}26)$$

Experience has shown that tightening the convergence criterion (that is reducing the tolerance in equation (5-25)) does not result in any significant change in the final values of the temperatures, liquid and vapour flowrates and compositions.

The weighting factor t used in step (viii) is chosen as follows[17]. First an initial value of t, $t^{(1)}$, is chosen as the smallest value of t (less than or equal to unity) which satisfies both equations (5-27) and (5-28):

$$T_j^k - \Delta T_{lim} \leqslant T_j^k + t\,\Delta T_j \leqslant T_j^k + \Delta T_{lim} \qquad (5\text{-}27)$$

$$j = 1 \rightarrow \text{NTOTL}$$

$$0.5\,V_j^k \leqslant V_j^k + t\,\Delta V_j \leqslant 2.0\,V_j^k \qquad (5\text{-}28)$$

$$j = 1 \rightarrow \text{NTOTL}$$

where $\Delta T_{lim}$ is chosen by the user with a default value of 60°F. If $t^{(1)}$ does not satisfy the condition that

$$[\text{CRIT}]^{k+1} < [\text{CRIT}]^k \qquad (5\text{-}29)$$

then a second weighting factor $t^{(2)} = 0.5t^{(1)}$ is used. Generally this procedure produces monotonic convergence.

# 6. USE OF THE MULTICOLUMN ALGORITHM

Application of the algorithm discussed in Chapter 5 will be demonstrated with examples involving three different systems of columns. Limitations of the algorithm will be identified.

## 6.1 Example Problems

Problem No. 1 is a thermally coupled distillation system which is depicted in Figure 7. A hydrocarbon feed is split into three products; a ($C_2 + C_3$) fraction, a $C_4$ fraction and a $C_5^+$ fraction. The problem specifications and initial assumptions are:

Feed Composition

| Component | Feed (moles/time) |
|---|---|
| ethane | 37.7 |
| propane | 2156.1 |
| i-butane | 400.5 |
| n-butane | 715.3 |
| i-pentane | 251.2 |
| n-pentane | 267.1 |
| hexane | 141.8 |
| octane | 110.3 |

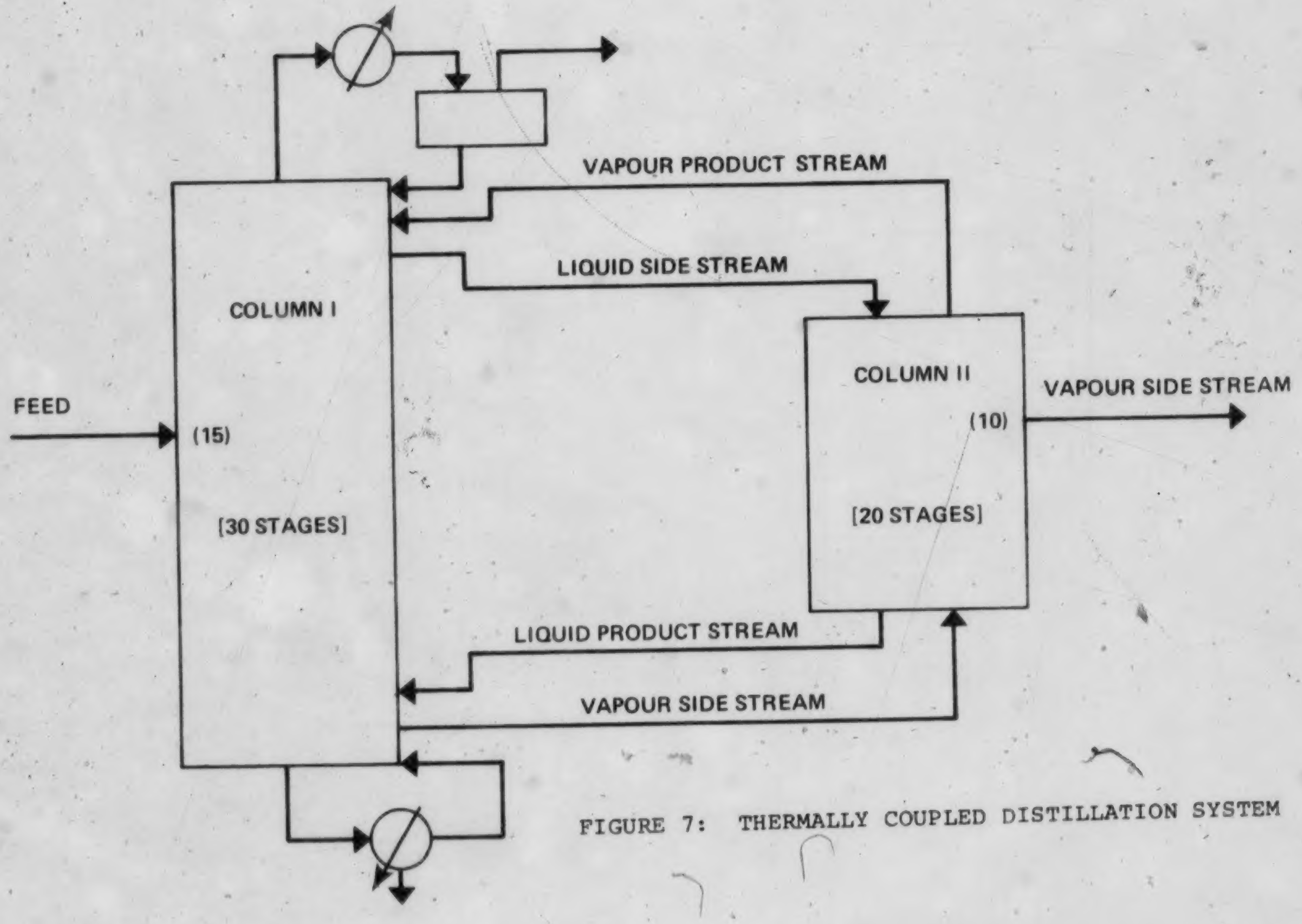

VAPOUR PRODUCT STREAM
LIQUID SIDE STREAM
COLUMN I
FEED
(15)
[30 STAGES]
COLUMN II
VAPOUR SIDE STREAM
(10)
[20 STAGES]
LIQUID PRODUCT STREAM
VAPOUR SIDE STREAM

FIGURE 7: THERMALLY COUPLED DISTILLATION SYSTEM

| | Column I | Column II |
|---|---|---|
| Number of equilibrium stages | 30 | 20 |
| Column pressure (psia) | 235 | 235 |
| Pressure drop per stage (psia) | 0 | 0 |

Feed stage number = 15

Feed conditions - temperature = 150°F

pressure = 235 psia

Vapour side stream leaves stage 40 (stage 10 of of column II)

Quantity = 1209.6 moles

The interlinked streams are as follows (see Figure 7)

| Type of Stream | Leaving Stage Number | Entering Stage Number | Quantity (moles/time) |
|---|---|---|---|
| Liquid sidestream | 5 | 31 | 2500 |
| Vapour sidestream | 25 | 50 | 3000 |
| Vapour product | 31 | 5 | a variable |
| Liquid product | 50 | 25 | a variable |

For column I the additional specifications are:

Reboiler vapour = 6850 moles/time

Reflux ratio = 2.50

Partial condenser

Equilibrium and enthalpy data were obtained using the Chao-Saeder correlation[5]. Details of the evaluation of the required partial derivatives have been given by Ishii[17].

The initial assumptions are as follows:

| Stage | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 122 | 2207.2 |
| 2 | 124 | 7725.4 |
| 3 | 126 | 7650 |
| 4 | 130 | 7600 |
| 5 | 134 | 7550 |
| 6 | 138 | 5000 |
| 7 | 142 | 5000 |
| 8 | 144 | 5000 |
| 9 | 146 | 5000 |
| 10 | 148 | 5000 |
| 11 | 150 | 5000 |
| 12 | 152 | 5000 |
| 13 | 154 | 5000 |
| 14 | 156 | 5000 |
| 15 | 164 | 5000 |
| 16 | 172 | 4800 |
| 17 | 180 | 4800 |
| 18 | 188 | 4800 |
| 19 | 196 | 4800 |
| 20 | 204 | 4800 |
| 21 | 212 | 4800 |
| 22 | 220 | 4800 |
| 23 | 228 | 4800 |
| 24 | 240 | 4800 |
| 25 | 252 | 4800 |
| 26 | 264 | 7500 |
| 27 | 276 | 7500 |
| 28 | 288 | 7500 |
| 29 | 300 | 7500 |
| 30 | 325 | 6850 |
| 31 | 137 | 2200 |
| 32 | 145 | 2200 |
| 33 | 153 | 2200 |
| 34 | 161 | 2200 |
| 35 | 173 | 2200 |
| 36 | 185 | 2200 |
| 37 | 197 | 2200 |
| 38 | 205 | 2200 |
| 39 | 213 | 2200 |
| 40 | 221 | 2200 |
| 41 | 229 | 3100 |
| 42 | 237 | 3100 |

(continued)

| Stage | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 43 | 242 | 3100 |
| 44 | 244 | 3100 |
| 45 | 246 | 3100 |
| 46 | 248 | 3100 |
| 47 | 250 | 3100 |
| 48 | 252 | 3100 |
| 49 | 254 | 3100 |
| 50 | 256 | 3100 |

## Problem No. 2

This problem is an extractive distillation system which separates an acetone-acetonitrile mixture using water as solvent. The system is depicted in Figure 8. The extraction column is taken from a paper by Ishikawa and Hirata[19]. Difficulty in choosing suitable values for the reflux ratio, number of stages and amount of reboiler vapour, such that the solvent is recovered in a single tower, motivated the use of two solvent recovery towers.

Detailed specifications of the problem are:

| Component | Solvent Circulation Rate (moles/time) | Feed (moles/time) |
|---|---|---|
| Acetone | - | 90.0 |
| Acetonitrile | - | 10.0 |
| Water | 200.0 | - |

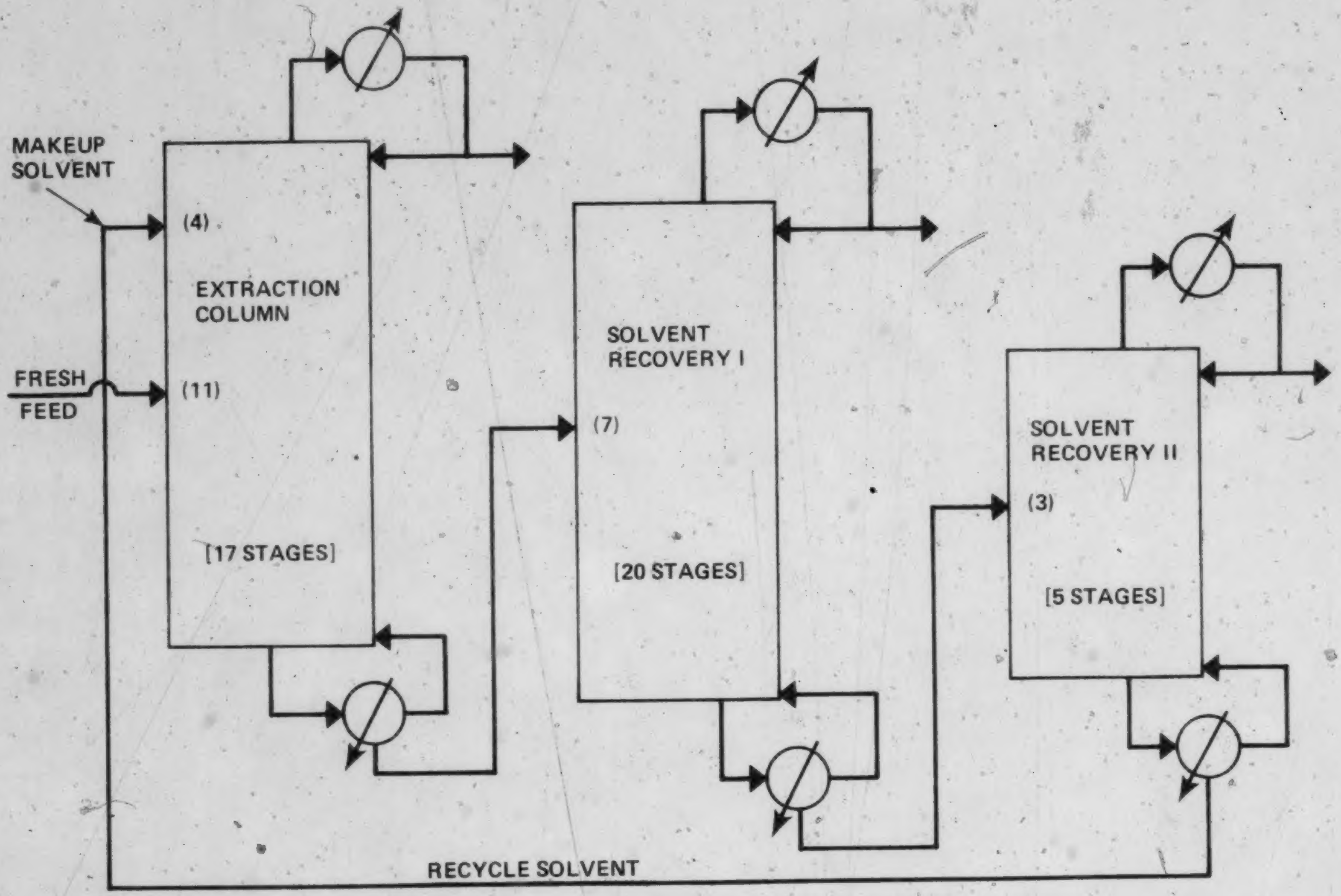

MAKEUP SOLVENT
FRESH FEED
(4)
EXTRACTION COLUMN
(11)
[17 STAGES]
SOLVENT RECOVERY I
(7)
[20 STAGES]
SOLVENT RECOVERY II
(3)
[5 STAGES]
RECYCLE SOLVENT

FIGURE 8: EXTRACTIVE DISTILLATION SYSTEM

| | Extraction Column | Solvent Recovery Towers I | Solvent Recovery Towers II |
|---|---|---|---|
| Number of equilibrium stages | 17 | 20 | 5 |
| Column pressure (psia) | 14.7 | 14.7 | 14.7 |
| Pressure drop per stage (psia) | 0.0 | 0.0 | 0.0 |
| Reflux ratio | 3.0 | 2.0 | 10.0 |
| Reboiler vapour (moles/time) | 185.0 | 135.0 | 95.0 |
| Condenser | total | total | total |

Fresh feed stage = 11

Feed conditions: bubble point temperature

pressure = 14.7 psia

| Type of Interlinked Stream | Leaving Stage Number | Entering Stage Number | Quantity |
|---|---|---|---|
| Liquid product | 17 | 24 | variable |
| Liquid product | 37 | 40 | variable |
| Liquid product | 42 | 4 | variable |

Equilibrium K-ratios are provided by vapour pressures and activity coefficients, the latter being given by Margules third order equations. Enthalpy data is evaluated using average specific heats and latent heats of vapourization. Details of the above evaluations and of the calculation of partial derivatives are given in Appendix 5.

The initial assumptions are as follows:

| Stage No. | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 134 | 0 |
| 2 | 135 | 200 |
| 3 | 136 | 200 |
| 4 | 137 | 200 |
| 5 | 138 | 200 |
| 6 | 139 | 200 |
| 7 | 140 | 200 |
| 8 | 141 | 200 |
| 9 | 142 | 200 |
| 10 | 143 | 200 |
| 11 | 144 | 200 |
| 12 | 145 | 200 |
| 13 | 146 | 200 |
| 14 | 147 | 200 |
| 15 | 148 | 200 |
| 16 | 149 | 200 |
| 17 | 150 | 185 |
| 18 | 138 | 0 |
| 19 | 143 | 165 |
| 20 | 148 | 165 |
| 21 | 153 | 165 |
| 22 | 158 | 165 |
| 23 | 163 | 165 |
| 24 | 166 | 165 |
| 25 | 168 | 165 |
| 26 | 170 | 165 |
| 27 | 172 | 165 |
| 28 | 180 | 165 |
| 29 | 180 | 165 |
| 30 | 180 | 165 |
| 31 | 180 | 165 |
| 32 | 180 | 165 |
| 33 | 180 | 165 |
| 34 | 185 | 165 |
| 35 | 190 | 165 |
| 36 | 195 | 165 |
| 37 | 200 | 135 |
| 38 | 150 | 0 |
| 39 | 180 | 110 |
| 40 | 200 | 110 |
| 41 | 205 | 110 |
| 42 | 210 | 95 |

## Problem No. 3

This problem involves a typical amine sweetening system, using MEA as solvent. The system is the same as that depicted in Figure 1. Problem specifications are:

### Composition of Feed

| Component | Sour Gas (moles/time) |
|---|---|
| $H_2S$ | 35.7 |
| $CO_2$ | 39.5 |
| MEA | - |
| $H_2O$ | 5.0 |
| hydrogen | 500.0 |
| nitrogen | 5000.0 |
| methane | 4000.0 |
| ethane | 2500.0 |
| propane | 900.0 |
| n-butane | 89.0 |
| i-butane | 89.0 |

| | Contactor | Regenerator |
|---|---|---|
| Number of ideal stages | 10 | 14 |
| Pressure, psia | 250.0 | 28.0 |
| Pressure drop per stage | - | 0.33 |

Condenser conditions - temperature = 120°F
pressure = 27 psia
partial condenser

Reboiler duty = 13.8 MM BTU/time.

Amount of amine in lean amine stream = 127.35 moles/time.

Solution strength (wt. pct.) = 15.3

Total flowrate of semilean amine stream = 2550 moles/time

Semilean stream goes from stage 17 to stage 5

Rich amine enters stage 12

| Stream | Entering Temperature (°F) | Entering Pressure (psia) |
|---|---|---|
| Sour gas feed | 90 | 250 |
| Lean amine | 110 | 250 |
| Rich amine | 190 | 100 |
| Semilean amine | 100 | 250 |

Equilibrium and enthalpy data were provided by the correlation of Nasir[35].

Initial assumptions for the stage variables are:

| Stage No. | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 1 | 100 | 13090 |
| 2 | 100 | 13090 |
| 3 | 100 | 13090 |
| 4 | 100 | 13090 |
| 5 | 100 | 13090 |
| 6 | 100 | 13090 |
| 7 | 100 | 13090 |
| 8 | 100 | 13090 |
| 9 | 100 | 13090 |
| 10 | 110 | 13090 |
| 11 | 120 | 80 |
| 12 | 230 | 240 |
| 13 | 232 | 500 |
| 14 | 234 | 600 |
| 15 | 236 | 615 |
| 16 | 238 | 630 |

(continued)

| Stage No. | Temperature (°F) | Vapour Rate (moles/time) |
|---|---|---|
| 17 | 240 | 645 |
| 18 | 242 | 660 |
| 19 | 244 | 675 |
| 20 | 246 | 690 |
| 21 | 248 | 705 |
| 22 | 250 | 720 |
| 23 | 252 | 735 |
| 24 | 254 | 750 |

Estimated reflux ratio = 2.0

## 6.2 Results and Discussion

Computer printouts for the example problems are given in Appendix 6. Convergence characteristics and CPU times for each problem are summarized in Table 8.

TABLE 8: CONVERGENCE CHARACTERISTICS AND CPU TIMES FOR LINKED COLUMN EXAMPLE PROBLEMS

| Thermally Coupled Distillation System | | Extractive Distillation System | | Amine Treating System | |
|---|---|---|---|---|---|
| Iter. No. | [CRIT] | Iter. No. | [CRIT] | Iter. No. | [CRIT] |
| 0 | 2.32 | 0 | 14.64 | 0 | 0.16 |
| 1 | $0.62\cdot10^{-2}$ | 1 | 26.89 | 1 | $0.19\cdot10^{-1}$ |
| 2 | $0.24\cdot10^{-2}$ | 4 | 0.49 | 2 | $0.49\cdot10^{-2}$ |
| 3 | $0.13\cdot10^{-2}$ | 7 | 0.12 | 3 | $0.42\cdot10^{-2}$ |
| 4 | $0.75\cdot10^{-3}$ | 10 | $0.30\cdot10^{-1}$ | 4 | $0.17\cdot10^{-2}$ |
| 5 | $0.11\cdot10^{-3}$ | 13 | $0.23\cdot10^{-2}$ | 5 | $0.44\cdot10^{-4}$ |
| 6 | $0.53\cdot10^{-4}$ | 16 | $0.46\cdot10^{-3}$ | 6 | $0.20\cdot10^{-4}$ |
| 7 | $0.55\cdot10^{-5}$ | 19 | $0.20\cdot10^{-3}$ | | |
| | | 21 | $0.15\cdot10^{-4}$ | | |
| CPU Time (secs) | | CPU Time (secs) | | CPU Time (secs) | |
| 24.1+ | | 21.2+ | | 4.7+ | |

---

+ On an Amdahl 470 V/6

### 6.2.1 Evaluation of the Algorithm

Important factors in evaluating the linked column algorithm include: ease and rate of convergence, limitations of the algorithm and the computer storage and time requirements.

The example problems show that with reasonable initial assumptions the program is able to converge. However, experience has shown that more iterations may be needed where the assumptions are far removed from solution. This is not usually so in the solution of individual columns. In addition, convergence is not always monotonic with the linked column algorithm (see especially iterations 0 and 1 for the extractive distillation problem in Table 8). Non-monotonic behaviour occurs mostly in the early iterations and when large corrections to temperatures, vapour flow rates and liquid compositions are generated. More work on the choice of the weighting factor used in equations (5-21) to (5-23) may then help to increase the rate of convergence. Despite the non-monotonic behaviour, the program has demonstrated robustness in converging for a wide range of initial assumptions.

One limitation of the algorithm is that it encounters difficulty in converging with some specifications. The specifications that present problems are the following:

(i) reflux ratio and total amount of top product (distillation)

(ii) reflux ratio and total amount of bottom product (distillation)

(iii) total amount of top product (reboiled absorber)

(iv) total amount of bottom product (reboiled absorber)

Cases (i) and (ii) are specifications made in place of the condenser duty and reboiler duty, and cases (iii) and (iv) are those made instead of the reboiler duty.

The difficulties encountered with the above specifications are mostly related to the occurrence of a singular matrix in the linearized material balance equation (cases (i), (ii) and (iv)). It is unclear why case (iii) does not work, although Harclerode and Gentry[14] indicate their algorithm is restricted to cases where symmetrical specifications are made, and this restriction could also apply to case (iii). On the other hand, both cases (ii) and (iv) are symmetrical, yet neither works. Thus restrictions on the present algorithm differ from those given by Harclerode and Gentry[14], as some of both symmetrical (cases (ii) and (iv)) and non-symmetrical (cases (i) and (iii)) specifications do not produce a converged solution. Note that the difficulties just discussed only arise for the linked column program.

In summary, specifications that are successfully handled are the following, where one each of (a) and (b) is selected for a distillation column, and one of (b) for a reboiled absorber:

(a) reflux ratio, condenser temperature, condenser duty

(b) amount of reboiler vapour, reboiler duty.

For a given number of stages, more computer storage and CPU time per iteration are required by the algorithm than for the solution of a single column. Most of the increase in CPU time requirements is related to the elimination of the $\overline{\Delta L}$ matrix from the linearized equations and to the handling of off-tridiagonal elements. No special techniques were introduced to make the matrix manipulations more efficient; thus some savings in the times quoted in Table 8 could be achieved by utilizing more fully the block tridiagonal nature of the matrices. In particular, a number of multiplications by zero can be eliminated without the need for time consuming comparisons. Even without any refinements to the handling of the matrix equations the CPU times required per iteration are very favourable.

Finally, the handling of intercooling or heating of interlinked streams is a useful capability. Change of phase in the heating or cooling is not presently accounted for, but theoretically this could be readily incorporated as the additional requirement is merely a flash calculation on the entering stream to determine its condition and enthalpy.

### 6.2.2 Example Problem 1

The configuration used for the thermally coupled problem differs from that suggested by Stupin and Lockhart[41] in that the feed enters the reboiled column and the side vapour product leaves the other column, rather than the reverse being true. For the number of stages, reboiler duty and quantities of interlinked side vapour and side liquid streams, the configuration used in the example produced a better separation of the feed into the desired product fractions.

Four runs were performed of Problem 1, with essentially the same reboiler duty and using different specifications on the reboiled column. Both system configurations were used. A brief comparison of the results is given in Table 9, where 'a' denotes the present configuration and 'b' that used by Stupin and Lockhart[41]. A fuller analysis of the thermally coupled system would involve determination of the energy savings it offers over the conventional system of employing a reboiler on both columns.

TABLE 9: COMPARISON OF RUNS FOR THERMALLY COUPLED DISTILLATION PROBLEM.

| Configuration | Specified Variables | Percent Recovery of: $C_3$ | $C_4$'s | $C_5$'s | Reflux Ratio | Condenser Temp (°F) | No. of Iterations |
|---|---|---|---|---|---|---|---|
| a | $V_{NB}$, R | 98.1 | 93.4 | 75.3 | 2.5 | 121.78 | 7 |
| a | $Q_{NB}$, $T_{NT}$ | 98.1 | 93.5 | 75.6 | 2.51 | 121.71 | 5 |
| b | $Q_{NB}$, $T_{NT}$ | 77.6 | 65.4 | 99.5 | 3.53 | 121.71 | 5 |
| b | $Q_{NB}$, R | 80.7 | 64.1 | 84.5 | 2.5 | 137.71 | 4 |

### 6.2.3 Example Problem 2

For the extractive distillation problem, some changes were made to the equations presented in Chapter 5 to account for the makeup solvent stream. If n is the entering stage number and NB the leaving stage number of the recycle solvent, the following changes are made to the equations about stage n.

(i) In equation (5-1), $\psi_{C,i,k}$ for component i in the solvent equals $L'_{NB}\ x'_{i,NB}$

(ii) In equation (5-2), $\psi_{E,k}$ for the solvent equals $L'_{NB}\ h'_{NB}$

(iii) In equation (5-3), $\psi_{M,k}$ is $L'_{NB}$ for the solvent where: $L'_{NB} = L_{NB}$ + makeup solvent

$$x'_{i,NB} = \frac{L_{NB}\, x_{i,NB}}{L'_{NB}} \qquad \begin{array}{l} i = 1 \rightarrow NCP \\ i \neq ns \end{array}$$

$$x'_{ns,NB} = \frac{\text{solvent circulation rate}}{L'_{NB}}$$

$h'_{NB}$ is evaluated at the specified entering temperature of the solvent for liquid compositions $x'_{i,NB}$.

$L'_{NB}$ is calculated as a known quantity at each iteration from the equation

$$L'^{(k+1)}_{NB} = [L^{(k)}_{NB} + \Delta L^{(k)}_{NB}]\ (1 - x_{ns,NB})$$
$$+ \text{(specified) solvent circulation rate} \qquad (6\text{-}1)$$

Then in the linearized equations, namely (5-4), (5-5) and (5-6), no terms in $\Delta x_{i,NB}$, $\Delta L_{NB}$ or $\Delta T_{NB}$ appear in the equations around stage n.

In the final solution the required makeup of solvent equals the difference between the circulation rate (moles/time) and the moles of solvent in the stream leaving stage NB. The makeup of water in problem 2 is then 19.5 moles/time.

Alternatively to the above procedure, the makeup of solvent could be calculated at each iteration as the total amount of solvent lost in streams leaving the system. Then $L'_{NB}$ is given directly from the sum of $L_{NB}$ and the makeup solvent. The methods produce equivalent results, although in the former a check should be made that the solvent material balance around the system closes. This is so for the example problem, to the accuracy of the printed results.

In the linearized equations, the partial derivatives with respect to composition were set equal to zero, even though the equilibrium K-ratios are strongly composition dependent. This did not prevent a converged solution being reached. In fact, when the partials were included, a solution was not achieved for the example problem. The omission of the partials does not affect the rigour of the solution as the K-ratios are calculated exactly as functions of composition at each iteration.

For a solvent recovery tower, it is difficult to choose appropriate values for the number of stages, the reflux ratio and the amount of reboiler vapour such that the desired separation of the solvent from other components is achieved. This difficulty largely motivated the use of two solvent recovery towers, as a number of attempts at using a single recovery tower failed to produce a converged result. The separation achieved in problem 2 appears quite reasonable as the top product from the extraction column is 92.5% acetone and contains only 90 ppm acetonitrile, while 95% of the acetonitrile is recovered in the top product of solvent recovery tower 1. The second solvent recovery tower removes the remaining acetonitrile and produces an overhead product containing 5.26% acetonitrile and only 2 ppm acetone.

In addition the use of two solvent recovery towers demonstrates that the algorithm can solve systems of more than two columns.

### 6.2.4 Example Problem 3

In the case of the amine system, modifications to the linearized equations are needed because the quantities of amine and water in the lean amine are specified. The changes are the same in form as those for the extraction problem, with the quantities $L'_{NB}$, $x'_{i,NB}$ and $h'_{NB}$ being calculated as follows, where subscripts 3 and 4 denote amine and water respectively.

$$L'^{(k+1)}_{NB} = [L^{(k)}_{NB} + \Delta L^{(k)}_{NB}]\,(1-x_{3,NB}-x_{4,NB}) + \text{(moles amine + moles water) in the lean amine} \qquad (6\text{-}2)$$

$$x'_{i,NB} = \frac{L_{NB}\,x_{i,NB}}{L'_{NB}} \qquad i = 1,2,5 \rightarrow NCP \qquad (6\text{-}2\text{-}a)$$

$$x'_{3,NB} = \frac{\text{moles amine in lean amine}}{L'_{NB}} \tag{6-2-b}$$

$$x'_{4,NB} = \frac{\text{moles water in lean amine}}{L'_{NB}} \tag{6-2-c}$$

Moles water in lean amine

$$= (\text{moles amine in lean amine}) \left(\frac{XM_3}{XM_4}\right) \left(\frac{100-wt}{wt}\right) \tag{6-2-d}$$

where wt $\equiv$ weight percent of amine in solution,

and $XM_i$ is the molecular weight of i.

$h'_{NB}$ is evaluated at the specified lean amine temperature for liquid compositions $x'_{i,NB}$.

The required makeup of amine and water is then the difference between the specified moles of each in the lean amine and the moles in the bottoms liquid product from the regenerator. For problem 3 the makeups are 0.10 moles amine and 54.3 moles water.

Each interlinked stream undergoes heat exchange before entering its destined stage. It is usual to control the entering temperatures of the lean, semilean and rich amine streams[30]; thus the entering temperatures are specified. If the stream leaves stage k and enters stage n, no terms in $\Delta T_k$ appear in the linearized enthalpy balance equation (5-5) around stage n.

## 6.3 Application to the Design of Amine Treating Systems

It is the intention of this section to very briefly demonstrate two particular design considerations that can be investigated using the linked column algorithm, namely the option of using a split flow system and the determination of a suitable reboiler steam rate to achieve a desired lean amine residual.

### 6.3.1 The Split Flow System Option

This option is claimed to have particular advantages for feed streams containing over 30 percent acid gas[30]. Thus a feed containing 30% $H_2S$ and 3% $CO_2$ was used. The basic system is the same as that depicted in Figure 1, with the omission of the semilean stream for the non-split flow case. Specifications for the columns are the same as in problem 3, except for the following changes:

Sour Gas Feed

| Component | Feed (moles/time) |
|---|---|
| $H_2S$ | 1500 |
| $CO_2$ | 150 |
| $H_2O$ | 5 |
| $N_2$ | 1000 |
| $CH_4$ | 1500 |
| $C_2H_6$ | 800 |
| $C_3H_8$ | 45 |

| | Non-Split Flow | Split Flow |
|---|---|---|
| Amount of amine [illegible] lean amine stream (moles/time) | 3760 | 2500 |
| Reboiler duty (MM BTU/time) | 225 | 195 |
| Total amount of semilean amine stream (moles/time) | - | 30,000 |

The total quantity of amine in the system is then the same for the two cases. Table 10 lists the sweet gas $H_2S$ and $CO_2$ compositions, the quantities of acid gas in the regenerated lean amine and the regenerator reflux ratio for the split flow and non-split flow (conventional) problems. The split flow configuration produces the sweeter overheads product while using less steam in the reboiler.

Thus the results of this example support the contention that for gas streams with a high acid gas content, a split flow system is advantageous because of the saving in operation costs resulting from reduced heat requirements in the reboiler. In a similar fashion the linked column algorithm can be used to determine whether the advantage holds for feeds with other acid gas contents.

### TABLE 10

### COMPARISON OF RESULTS GIVEN BY SPLIT FLOW AND CONVENTIONAL CONFIGURATIONS

| VARIABLE | | CONVENTIONAL | SPLIT FLOW |
|---|---|---|---|
| Sweet Gas Composition (ppm) | $H_2S$ | 19.2 | 16.0 |
| | $CO_2$ | 0.21 | 0.19 |
| Lean Amine Residuals (moles/time) | $H_2S$ | 137.6 | 83.1 |
| | $CO_2$ | 62.5 | 42.1 |
| Reflux Ratio | | 2.25 | 1.37 |
| Reboiler Duty (MM BTU/time) | | 225 | 195 |

### 6.3.2 Choice of a Stripping Stream Rate to Achieve a Given Lean Amine Residual

Fitzgerald and Richardson[9] used data from a number of operating units to prepare plots relating the lean amine residuals of $H_2S$ and $CO_2$ to the $H_2S/CO_2$ feed ratio and to the steam rate in the reboiler. The program can be used to generate similar information subject to limitations or inaccuracies in the equilibrium data and stage efficiencies.

To demonstrate this use of the program, a number of runs were made using the same operating conditions as in example problem 3, with the reboiler duty and $H_2S/CO_2$ feed ratio as variables. In all cases the total quantity of acid gas in the sour gas feed was 75.2 moles. An effective quantity of circulating amine, which includes the quantity in both the lean and semilean amine streams, was used. This was in order to account for the split-flow configuration.

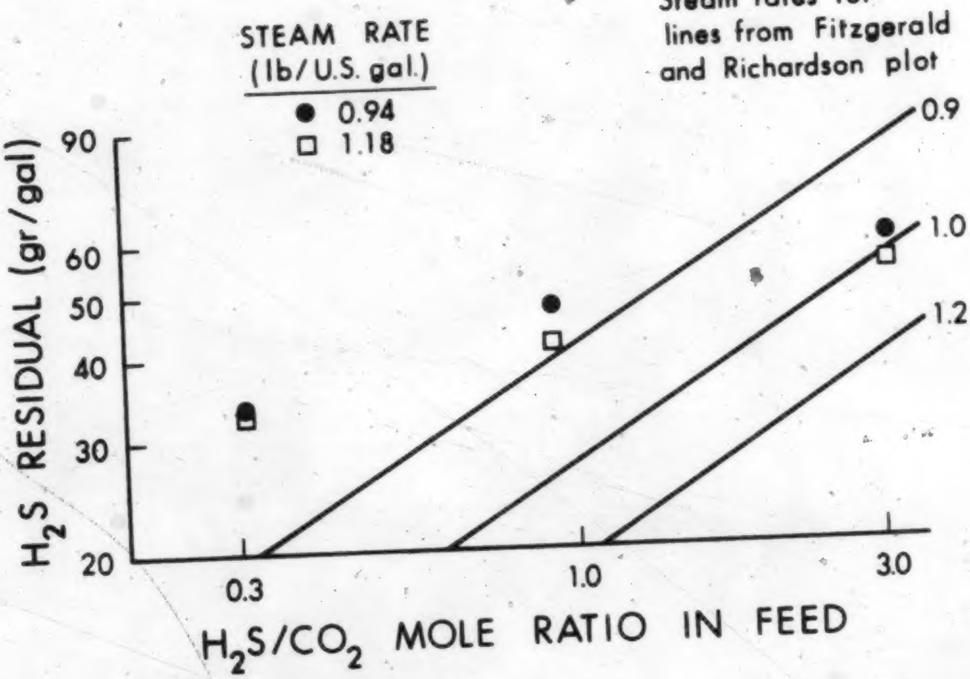
Two steam rates and three $H_2S/CO_2$ feed ratios were used. The resulting $H_2S$ and $CO_2$ residuals in the lean amine are given in Table 11.

TABLE 11: $H_2S$ and $CO_2$ LEAN AMINE RESIDUALS FOR DIFFERENT REBOILER STEAM RATES AND ACID GAS RATIOS IN THE FEED.

| $H_2S/CO_2$ Mole RATIO IN FEED | $H_2S$ RESIDUALS* | | $CO_2$ RESIDUALS* | |
|---|---|---|---|---|
| | Steam Rate + | | Steam Rate + | |
| | 0.94 | 1.18 | 0.94 | 1.18 |
| 0.3 | 32.8 | 31.8 | 140.7 | 127.7 |
| 0.9 | 46.7 | 40.9 | 120.6 | 105.4 |
| 3.0 | 58.2 | 52.5 | 91.4 | 83.8 |

* grains per gallon of amine in the system

+ lbs. of 55 psia steam per gallon of amine in the system.



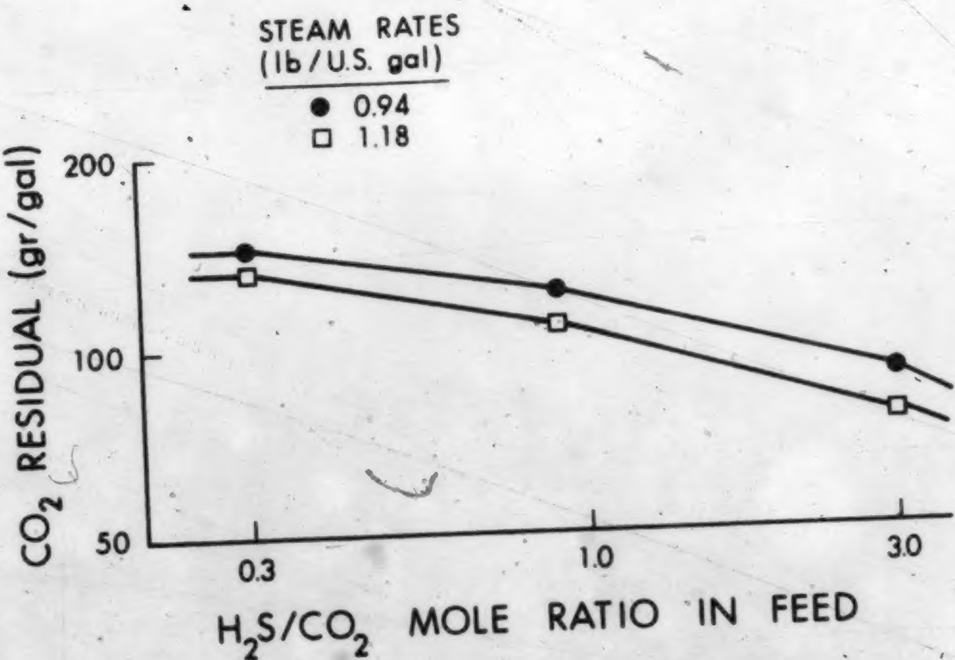


FIGURE 9: ACID GAS LEAN AMINE RESIDUALS VERSUS ACID GAS FEED RATIO AT DIFFERENT STEAM RATES

The points are plotted on log-log plots as shown in Figure 9. For comparison the straight lines published by Fitzgerald and Richardson[9] are shown on the $H_2S$ plot. The experimental points lie above those given by interpolating between the lines. Thus the program predicts poorer stripping than indicated by Fitzgerald and Richardson[9].

In the case of $CO_2$ the points lie well below the published curves, which give residuals of between about 450 and 1000 gr/gal for the range of acid gas feed ratios used here. However, the same trend is displayed, namely a decreasing $CO_2$ residual with increasing acid gas feed ratio. The displacement is largely the result of inadequacies in equilibrium data and the use of equilibrium stages rather than actual stages (which incorporate stage efficiencies).

It is postulated that if an adequate set of stage efficiencies were used, the experimental lines would lie much closer to those of Fitzgerald and Richardson[9]. In fact a possible means of estimating the stage efficiencies could be the choice of a set of values that causes the predicted points to lie on the published lines. It should be remembered however, that the published lines represent smoothed data from a number of operating plants. Therefore it seems more reasonable to concentrate on improvements to the fundamental estimation of stage efficiencies rather than to rely on empirical fitting.

A combination of plots such as Figure 9 and Figure 3 provides a method for the estimation of the steam rate required in the regenerator to meet a given overheads specification in the sweet gas. This is a very useful application of the linked column algorithm.

# 7. CONCLUSIONS

The computational model that has been developed is fast and efficient in providing design data for amine contactors and regenerators. The model can handle data from any given correlation of the solubilities of $H_2S$ and $CO_2$ in amine solutions. Use of the model provides values for important design variables, such as the regenerator steam load and the amine circulation rate. In addition the desirability of using a semilean amine stream in the contactor can be determined.

The incorporation of vapourization stage efficiencies into the model equations has been discussed. These efficiencies can be calculated from fundamental rate data and the values obtained indicate that the consideration of efficiencies is important for an accurate design. However, there is a need for more work to obtain better rate data on the absorption process before reliable estimates of the vapourization efficiencies can be made.

The extension of the single column computational model to the solution of systems of columns has been formulated, and the algorithm successfully tested on three systems, namely a thermally coupled distillation system, an extractive distillation system and an amine treating system. Convergence is not dependent on the accuracy of the initial assumptions, although the rate of convergence may differ. More work is suggested to clarify the influence of the weighting factor on the rate of convergence.

The partial derivatives with respect to composition may be omitted for some problems without affecting convergence. However they must be employed for amine problems.

Some specifications will not work with the algorithm. In most cases this is a result of singular matrices occurring in the solution process. In other cases, the reason is unclear, but it may be related to the restriction quoted by Harclerode and Gentry, which demands that specifications be symmetrical.

For a given size of problem, computer storage and CPU time requirements are larger than for the single column algorithm, but are still favourable. Improvements in the efficiency of the matrix handling routines will reduce the time requirement.

The use of the linked column algorithm in the simultaneous design of contactor and regenerator can provide data on a complete design that meets given requirements on the sweet gas.

Further work on the algorithm is suggested in the following areas:

(i) application to configurations involving lean oil absorbers.

(ii) a full determination of where $\partial K/\partial x$ is necessary and where not

(iii) the incorporation of vapourization efficiencies in the design of complete amine systems.

# NOMENCLATURE

| | |
|---|---|
| a | ratio of the un-ionized alkanolamine activity to the activity of water |
| a | interfacial area per volume of column |
| a,b,c | elements in matrix |
| a" | interfacial area per area of tray |
| A,B | functions in equations (2-4) and (2-5) |
| A,B,C,D,E | constants in ideal gas enthalpy correlation |
| $\bar{A},\bar{B}$ | matrices |
| AL,BL,CL | constants in latent heat correlation |
| bo | bulk phase concentration |
| c | component material imbalance function, defined by equations (3-2) and (5-1) |
| $c'_o$ | interfacial concentration |
| $\bar{C}$ | column vector |
| CRIT | convergence criterion, defined by equation (5-26) |
| D | diffusivity |
| $\bar{D}$ | matrix |
| e | vapourization stage efficiency |
| E | energy imbalance function, defined by equations (3-3) and (5-2) |
| $E_{MV}$ | Murphree vapour stage efficiency |

## NOMENCLATURE (continued)

| | |
|---|---|
| F | molar feed rate |
| $\overline{F},\overline{G},\overline{H}$ | matrices |
| h | enthalpy of liquid |
| hc | average heat capacity |
| H | enthalpy of vapour |
| H | Henry's Law coefficient |
| $\Delta H_{sol}$ | enthalpy of solution |
| I | enhancement factor |
| $\overline{I}$ | identity matrix |
| $k_g a$ | gas phase mass transfer coefficient |
| $k_G$ | gas phase mass transfer coefficient, defined by equation (4-1) |
| $k_L$, $k_L^o$ | liquid phase mass transfer coefficients, with and without chemical reaction. |
| K | equilibrium K-ratio, or equilibrium constant |
| $K_{OG}$ | overall mass transfer coefficient |
| L | molar liquid flow rate |
| $\overline{\Delta L}$ | column vector containing corrections to molar liquid flow rates |
| m | amine molality or molarity |
| M | overall material imbalance function, defined by equations (3-5) and (5-3) |

## NOMENCLATURE (continued)

| | |
|---|---|
| $\overline{M}$ | column vector |
| $n_1, n_2, n_3$ | bottom stage numbers of successive columns in three column system |
| NB | bottom stage of a column |
| NCP | number of components |
| NT | top stage of a column |
| NTOTL | total number of stages in a system of columns |
| p | pressure |
| $P_{CO_2}$ | $CO_2$ partial pressure |
| $P_{H_2S}$ | $H_2S$ partial pressure |
| $\overline{P}$ | matrix |
| q | stoichiometric coefficient |
| Q | heat duty |
| $\overline{Q}$ | matrix |
| R | gas constant |
| R | reflux ratio |
| $\overline{R}$ | matrix |
| S | summation imbalance, defined by equation (3-4) |
| S | cross sectional area of column, or volume of liquid on tray per area of tray |
| SL | molar flow rate of liquid side stream |
| SV | molar flow rate of vapour side stream |
| t | weighting factor |

## NOMENCLATURE (continued)

| | |
|---|---|
| $T$ | temperature |
| $\overline{\Delta T}$ | column vector containing temperature corrections |
| $u$ | volumetric gas flow per area of tray |
| $V$ | molar vapour flow rate |
| $\overline{\Delta V}$ | column vector containing corrections to molar vapour flow rates |
| $\overline{Va}$ | mean rate of absorption |
| wt | weight percent of amine in solution |
| $x$ | liquid composition |
| $\overline{\Delta x}$ | column vector containing corrections to liquid compositions |
| $X_{CO_2}$ | moles $CO_2$ per mole alkanolamine |
| $X_{H_2S}$ | moles $H_2S$ per mole alkanolamine |
| XM | molecular weight |
| $y$ | vapour composition |
| $z$ | feed composition |
| $z$ | function in equations (2-4) and (2-5), or depth of liquid on tray |

## NOMENCLATURE (continued)

### Greek Letters

| | |
|---|---|
| $\alpha$ | activity coefficient of water |
| $\gamma$ | average activity coefficient of an ion |
| $\Delta$ | "new value minus old value" |
| $\eta$ | composition dependent term in linearized equations arising from interconnected stream, defined in Table 6 |
| $\mu$ | viscosity |
| $\mu$ | temperature dependent term in linearized equations arising from interconnected stream, defined in Table 6 |
| $\rho$ | density |
| $\tau$ | overall molar flow rate dependent term in linearized equations arising from interconnected stream, defined in Table 6 |
| $\psi$ | contribution to material and energy balance equations from interlinked stream, defined in Table 5 |

NOMENCLATURE (continued)

Subscripts

| | |
|---|---|
| A | liquid phase |
| C | refers to component material balance |
| E | refers to energy balance |
| F | feed |
| G | gas phase |
| i | component number |
| int | interfacial value |
| j | stage number |
| k | leaving stage number of interlinked stream |
| lim | limit |
| L | liquid |
| M | refers to overall material balance |
| ns | component number of solvent |
| NB | bottom stage |
| NT | top stage |
| OD | containing off-tridiagonal elements (refers to a matrix) |
| T | total, or tridiagonal |
| vap | vapourization |

Superscripts

| | |
|---|---|
| e | equilibrium condition |
| k | iteration number |
| o | pure component, or ideal state |

# REFERENCES

1. American Petroleum Institute, "Technical Data Book - Petroleum Refining", 2nd ed., Washington, D.C. (1970).

2. Astarita, G., "Mass Transfer with Chemical Reaction", Elsevier, N.Y., (1967).

3. Billingsley, D.S., Can. J. Chem. Eng., 49, 672, (1971).

4. Carnahan, B., Luther, H.A. and Wilkes, J.O., "Applied Numerical Methods", John Wiley and Sons, N.Y., (1969).

5. Chao, K.C. and Saeder, J.D., AIChE Journal, 7, 598, (1961).

6. Chemical Engineers' Handbook, C. Perry ed., 4th ed., McGraw-Hill, N.Y., (1963).

7. Danckwerts, P.V., "Gas Liquid Reactions", McGraw-Hill, N.Y., (1970).

8. Danckwerts, P.V. and Sharma, M.M., Chem. Engr., 202, 244, Oct. (1966).

9. Fitzgerald, K.A. and Richardson, J.A., Oil and Gas Journal, 64, (43), 110, (1966)

10. Friday, J.R. and Smith, B.D., AIChE Journal, 10, 698, (1964).

11. Gas Conditioning Fact Book, The Dow Chemical Company, Midland, Michigan (1962).

12. Gentry, J.W., Can. J. Chem. Eng., 48, 451, (1970).

13. Hala, E., Wichterle, I., Polak, J. and Boublik, T., "Vapor, Liquid Equilibrium Data at Normal Pressures", Pergamon Press, (1968).

14. Harclerode, H. and Gentry, J.W., Can. J. Chem. Eng., 50, 253, (1972).

15. Holland, C.D., "Multicomponent Distillation", Prentice-Hall, Englewood Cliffs, N.J., (1963).

1[illegible] Holland, C.D., "Fundamentals and Modeling of Separation Processes", Prentice-Hall, Englewood Cliffs, N.J., (1975).

17. Ishii, Y., M.Sc. Thesis, University of Alberta, (1973).

18. Ishii, Y. and Otto, F.D., Can. J. Chem. Eng., 51, 601, (1973).

19. Ishikawa, T. and Hirata, M., J. of Chem. Eng., of Japan, 5, 125, (1972).

20. Jelinek, J., Hlavacek, V. and Krivsky, Z., Chem. Eng. Sci., 28, 1833, (1973).

21. Kent, R.L. and Eisenberg, B. "Equilibrium of $H_2S$ and $CO_2$ with MEA and DEA Solutions", Report presented at Gas Conditioning Conference, (1975).

22. Klyamer, S.D., Kolesnikova, T.L. and Rodin, Yu.A., Gazov. Prom., 18, (2), 44, (1973).

23. Kohl, A.L., AIChE Journal, 2, 264, (1956).

24. Kohl, A.L. and Riesenfeld, F.C., "Gas Purification", 2nd ed., Gulf Publishing Co., Houston, Texas, (1974).

25. Lawson, J.D., private communication.

26. Lee, J.I., Otto, F.D. and Mather, A.E., J. Chem. and Eng. Data, 17, 465, (1972).

27. idem, J. Chem. and Eng. Data, 18, 71, (1973).

28. idem, Can. J. Chem. Eng., 52, 803, (1974).

29. idem, Report presented at the CNGPA Research Seminar, Calgary, Alberta, (1972).

30. Maddox, R.N., "Gas and Liquid Sweetening", 2nd ed., John Campbell Press, (1974).

31. Murphree, E.V., Ind. Eng. Chem., 17, 747, (1925).

32. Nagiev, M.F., Chem. Eng. Progr., 53, (6), 297, (1957).

33. Naphtali, L.M., Chem. Eng. Progr., 60, (9), 70, (1964).

34. Nartker, T.A., Skrygley, J.M. and Holland, C.D., Can. J. Chem. Eng., 44, 217, (1966).

35. Nasir, P., M.Sc. Thesis, University of Alberta, (1975).

36. Petryschuk, W.F. and Johnson, A.I., Can. J. Chem. Eng., 46, 348, (1968).

37. Ravicz, A.E. and Norman, R.L., Chem. Eng. Progr. 60, (5), 71, (1964).

38. Rosen, E.M., Chem. Eng. Progr., 58, (10), 69, (1962).

39. Rowland, C.H. and Grens, E.A. II, Hydro. Proc., 50, (9), 201, (1971).

40. Shoeld, M., U.S. Patent 1,971,798 (1934).

41. Stupin, W.J. and Lockhart, F.J., Chem. Eng. Progr., 68, (10), 71, (1972).

42. Tomme, W.J. and Holland, C.D., Hydro. Proc. and Pet. Ref., 41, (6), 145, (1962).

43. Treybal, R.E., "Mass Transfer Operations", 2nd ed., McGraw-Hill, N.Y., (1968).

# APPENDIX 1

# ENTHALPIES OF SOLUTION OF $CO_2$ AND $H_2S$ IN MEA AND DEA SOLUTIONS

(KJ/MOLE GAS)

# APPENDIX 1

## Enthalpies of Solution of $CO_2$ and $H_2S$ In MEA And DEA Solutions. (KJ/Mole Gas)

(a) MEA[28]

| Acid Gas | Moles Acid Gas/Mole MEA | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 | 1.2 | 1.4 | 1.6 |
| $CO_2$ | 85.4 | 66.0 | 50.7 | 38.6 | 29.5 | 23.1 | - | - |
| $H_2S$ | 48.5 | 47.6 | 46.3 | 42.5 | 24.6 | 16.8 | 12.6 | 11.0 |

(b) DEA[26,27]

| Acid Gas | Normality of Solution | Moles Acid Gas/Mole DEA | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 | 1.2 | 1.4 |
| $CO_2$ | 0.5 | 57.7 | 53.0 | 44.3 | 37.3 | 31.5 | 27.2 | 23.5 |
| | 2.0 | 67.2 | 59.5 | 47.5 | 38.8 | 32.0 | 27.2 | 23.5 |
| | 3.5 | 76.3 | 65.4 | 50.3 | 40.0 | 32.4 | 27.3 | 23.5 |
| | 5.0 | 84.3 | 70.5 | 52.6 | 40.9 | 32.7 | 27.4 | 23.5 |
| | 6.5 | 90.7 | 73.7 | 54.2 | 41.5 | 32.9 | 27.4 | 23.5 |
| | 8.0 | 96.2 | 76.3 | 55.5 | 41.8 | 33.0 | 27.4 | 23.5 |
| $H_2S$ | 2.0,3.5 | 47.7 | 43.5 | 40.0 | 31.9 | 16.4 | 12.5 | 11.0 |

(c) Values of Kohl and Riesenfeld[24].

| | MEA | DEA |
|---|---|---|
| $CO_2$ | 84.5 | 66.9 |
| $H_2S$ | 63.7 | 40.5 |

# APPENDIX 2

# CONSTANTS IN CORRELATIONS FOR IDEAL GAS ENTHALPY AND LATENT HEAT OF VAPOURIZATION

## * APPENDIX 2 *

### CONSTANTS FOR IDEAL GAS ENTHALPY

| COMPONENT | A | B | C | D | E |
|---|---|---|---|---|---|
| H2S | 0.20844E+02 | 0.33672E+00 | -0.94100E-03 | 0.19442E+02 | 0.0 |
| CO2 | 0.14001E+02 | 0.67027E+00 | -0.87505E-02 | -0.85736E+01 | 0.0 |
| MEA | 0.60910E+01 | 0.25510E+01 | -0.28010E-01 | 0.0 | 0.50000E+03 |
| DEA | 0.76270E+00 | 0.29060E+01 | -0.45920E-01 | 0.0 | 0.50000E+03 |
| WATER | 0.40832E+02 | 0.36710E+00 | 0.61600E-03 | 0.34424E+02 | 0.10000E+04 |
| HYDROGEN | 0.34135E+03 | -0.17541E+00 | 0.23314E-01 | -0.12957E+03 | 0.0 |
| NITROGEN | 0.23700E+02 | 0.97640E-01 | 0.59490E-03 | 0.15603E+02 | 0.0 |
| METHANE | 0.36817E+02 | 0.20062E+01 | -0.38246E-02 | 0.46138E+02 | 0.74900E+02 |
| ETHANE | 0.14009E+02 | 0.31357E+01 | -0.30512E-01 | 0.43453E+02 | 0.16[illegible]80E+03 |
| PROPANE | 0.80382E+01 | 0.34907E+01 | -0.39606E-01 | 0.27530E+02 | 0.16617E+03 |
| NBUTANE | 0.82935E+01 | 0.34600E+01 | -0.40211E-01 | 0.30351E+02 | 0.15304E+03 |
| IBUTANE | 0.65259E+01 | 0.35927E+01 | -0.43014E-01 | 0.20257E+01 | 0.15569E+03 |
| C-5'S | 0.80231E+01 | 0.34488E+01 | -0.40567E-01 | 0.21828E+02 | 0.14921E+03 |
| C-6'S | 0.78175E+01 | 0.34444E+01 | -0.40883E-01 | 0.18712E+02 | 0.14398E+03 |
| C-7'S+ | 0.75021E+01 | 0.33420E+01 | -0.39902E-01 | 0.14124E+02 | 0.14134E+03 |

### CONSTANTS FOR LATENT HEAT CORRELATION

| COMPONENT | AL | BL | CL |
|---|---|---|---|
| MEA | 0.65000E+03 | -0.37230E+00 | 0.0 |
| DEA | 0.53200E+03 | -0.32500E+00 | 0.0 |
| WATER | 0.11622E+04 | 0.10015E+00 | -0.57198E-03 |

# APPENDIX 3

# INTERMEDIATE PARTIAL DERIVATIVES REQUIRED IN THE DERIVATION OF $\partial K/\partial x$ FOR $H_2S$ AND $CO_2$

# APPENDIX 3

## Intermediate Partial Derivatives Required In The Derivation Of ∂K/∂x For $H_2S$ And $CO_2$

(1) For $H_2S$ {see equations (3-25) and (3-26)}

(a) $$\alpha = \frac{x_4}{x_4 + x_3\left(1 + \frac{x_1}{x_3} + \frac{x_2}{x_3}\right)}$$

$$\frac{\partial\alpha}{\partial x_1} \doteq \frac{-x_4}{\left[x_4 + x_3\left(1 + \frac{x_1}{x_3} + \frac{x_2}{x_3}\right)\right]^2} \doteq -x_4 \qquad \text{(A3-1)}$$

(b) $$A = mx_1 - P_1 H_1$$

$$= mx_1 - (P_T K_1 x_1)H_1$$

$$\frac{\partial A}{\partial x_1} = m - P_T K_1 H_1 \qquad \text{(A3-2)}$$

(c) $\gamma = f(\mu)$ and $\mu = g(x_{H_2S})$

$$\frac{\partial\gamma}{\partial x_1} = \left(\frac{\partial\gamma}{\partial\mu}\right) \cdot \left(\frac{\partial\mu}{\partial x_1}\right) \qquad \text{(A3-3)}$$

(i)

$$\gamma = \begin{cases} 0.9023 - 1.996\mu - .068e^{-\mu} & (\mu \leq 0.1) \\ 0.3991 - 3.384 \times 10^{-3}\mu + 0.3242e^{-\mu} & (\mu > 0.1\text{-MEA}) \\ 0.3664 - 1.598 \times 10^{-2}\mu + 0.3444e^{-\mu} & (\mu > 0.1\text{-DEA}) \end{cases}$$

$$\frac{\partial\gamma}{\partial\mu} = \begin{cases} -1.996 + .068e^{-\mu} & (\mu \leq 0.1) \\ -3.384 \times 10^{-3} - 0.3242e^{-\mu} & (\mu > 0.1\text{-MEA}) \\ -1.598 \times 10^{-2} - 0.3444e^{-\mu} & (\mu > 0.1\text{-DEA}) \end{cases}$$

(A3-4)

(ii)

$$\mu = 0.5\, m_i\, z_i^2$$

$$= 0.5\,\{[RNH_3^+] + [OH^-] + [H^+] + [HS^-] + 4[S^{2-}]$$

$$+ [RNHCOO^-] + [HCO_3] + 4[CO_3^{2-}]\}$$

where $[HS^-] = A$ , $[RNHCOO^-] = z$

and $[H^+]$ and $[S^{2-}]$ can be neglected.

$$\frac{\partial\mu}{\partial x_1} = 0.5\left\{\frac{\partial[RNH_3^+]}{\partial x_1} + \frac{\partial[OH^-]}{\partial x_1} + \frac{\partial A}{\partial x_1} + \frac{\partial z}{\partial x_1} + \frac{\partial[HCO_3^-]}{\partial x_1} + 4\,\frac{\partial[CO_3^{2-}]}{\partial x_1}\right\} \qquad \text{(A3-5)}$$

Now $[RNH_3^+] = A + B$

$[HCO_3^-] = B - z$

Thus
$$\frac{\partial [RNH_3^+]}{\partial x_1} = \frac{\partial A}{\partial x_1} \qquad \text{(A3-6)}$$

$$\frac{\partial [HCO_3^-]}{\partial x_1} = -\frac{\partial z}{\partial x_1} \qquad \text{(A3-7)}$$

as B is independent of $x_1$.

$$\therefore \frac{\partial \mu}{\partial x_1} = \frac{\partial A}{\partial x_1} + 0.5\,\frac{\partial [OH^-]}{\partial x_1} + 2\,\frac{\partial [CO_3^{2-}]}{\partial x_1} \qquad \text{(A3-8)}$$

Now (1) $[OH^-] = \dfrac{K_i a\alpha^2 (m-z-A-B)}{\gamma^2 (A+B)}$

$$\therefore \frac{\partial [OH^-]}{\partial x_1} = \frac{1}{\gamma^2 (A+B)} \left\{ (m-z-A-B)\ 2K_i a\alpha \frac{\partial \alpha}{\partial x_1} - K_i a\alpha^2 \left[\frac{\partial z}{\partial x_1} + \frac{\partial A}{\partial x_1}\right] \right\} + \frac{(K_i a\alpha^2)(m-z-A-B)}{\gamma^2 (A+B)} \left\{ -\frac{2}{\gamma}\frac{\partial \gamma}{\partial x_1} - \frac{1}{(A+B)}\frac{\partial A}{\partial x_1} \right\} \qquad \text{(A3-9)}$$

(2)

$$[CO_3^{2-}] = \frac{K_{2y}\ [HCO_3^-]}{\gamma\ [H^+]}$$

$$= \frac{K_{2y}\gamma\ [OH^-][HCO_3^-]}{\alpha K_W}$$

$$\therefore \frac{\partial [CO_3^{2-}]}{\partial x_1} = \frac{K_{2y}}{K_W}\left\{ -\frac{\gamma}{\alpha}\ [OH^-]\ \frac{\partial z}{\partial x_1} + \frac{\gamma}{\alpha}\ [HCO_3^-]\ \frac{\partial [OH^-]}{\partial x_1} + [OH^-][HCO_3^-]\left(\frac{1}{\alpha}\ \frac{\partial \gamma}{\partial x_1} - \frac{\gamma}{\alpha^2}\ \frac{\partial \alpha}{\partial x_1}\right)\right\} \qquad \text{(A3-10)}$$

as $\frac{\partial [HCO_3^-]}{\partial x_1} = -\frac{\partial z}{\partial x_1}$ from equation (A3-7)

Solution for $(\frac{\partial \gamma}{\partial x_1})$ is iterative.

(d) $A = m-z-B-Sz/(B-z)$

where $S = K_i\ K_{1y}\ H_1/K_W\ K_M\ a$

$$\therefore f(z) = (m-z-A-B)(z-B) + Sz = 0 \qquad \text{(A3-11)}$$

$$\frac{\partial z}{\partial x_1} = -\frac{(\partial f/\partial x_1)_z}{(\partial f/\partial z)_{x_1}} \qquad \text{(A3-12)}$$

(i) $$\left(\frac{\partial f}{\partial x_1}\right)_z = (B-z)\ \frac{\partial A}{\partial x_1} \qquad \text{(A3-13)}$$

(ii)

$$\left(\frac{\partial f}{\partial z}\right)_{x_1} = m-A+S-2z \qquad \text{(A3-14)}$$

(e) $$\frac{\partial A}{\partial K_1} = -\ P_T\ x_1\ H_1 \qquad \text{(A3-15)}$$

(f) $$\frac{\partial z}{\partial K_1} = -\frac{(\partial f/\partial K_1)_z}{(\partial f/\partial z)_{K_1}} \qquad \text{(A3-16)}$$

(i) $$\left(\frac{\partial f}{\partial K_1}\right)_z = (B-z)\ \frac{\partial A}{\partial K_1} \qquad \text{(A3-17)}$$

(ii) $$\left(\frac{\partial f}{\partial z}\right)_{K_1} = m-A+S-2z \qquad \text{(A3-18)}$$

(2) For $CO_2$ {see equations (3-27) and (3-28)}

(a) $$\frac{\partial \alpha}{\partial x_2} = \frac{-x_4}{[x_4+x_3(1+\frac{x_1}{x_3}+\frac{x_2}{x_3})]^2} \doteqdot -x_4 \qquad \text{(A3-19)}$$

(b) $$B = mx_2 - P_T\ K_2\ x_2\ H_2$$

$$\frac{\partial B}{\partial x_2} = m - P_T\ K_2\ H_2 \qquad \text{(A3-20)}$$

(c) $$\frac{\partial \gamma}{\partial x_2} \doteqdot (\frac{\partial \gamma}{\partial \mu})(\frac{\partial \mu}{\partial x_2}) \qquad \text{(A3-21)}$$

(i) $\frac{\partial\gamma}{\partial\mu}$ - see equation (A3-4)

(ii) Using equation (A3-5) with $x_1$ replaced by $x_2$, and the relations:

$$\frac{\partial[RNH_3^{+}]}{\partial x_2} = \frac{\partial B}{\partial x_2}$$

and

$$\frac{\partial[HCO_3^{-}]}{\partial x_2} = \frac{\partial B}{\partial x_2} - \frac{\partial z}{\partial x_2}$$

one obtains -

$$\frac{\partial\mu}{\partial x_2} = \frac{\partial B}{\partial x_2} + 0.5\,\frac{\partial[OH^{-}]}{\partial x_2} + 2\,\frac{\partial[CO_3^{2-}]}{\partial x_2} \qquad \text{(A3-22)}$$

Now (1)

$$\begin{aligned}\frac{\partial[OH^{-}]}{\partial x_2} = {} & \frac{1}{\gamma^2(A+B)}\left\{(m-z-A-B)\;2K_i a\alpha\,\frac{\partial\alpha}{\partial x_2} - K_i a\alpha^2\left[\frac{\partial z}{\partial x_2} + \frac{\partial B}{\partial x_2}\right]\right\} \\ & + \frac{K_i a\alpha^2}{\gamma^2(A+B)}\,(m-z-A-B)\left\{-\frac{2}{\gamma}\,\frac{\partial\gamma}{\partial x_2} - \frac{1}{(A+B)}\,\frac{\partial B}{\partial x_2}\right\}\end{aligned} \qquad \text{(A3-23)}$$

(2)

$$\begin{aligned}\frac{\partial[CO_3^{2-}]}{\partial x_2} = \frac{K_2\gamma}{K_W}\Bigg\{ & \frac{\gamma}{\alpha}\,[OH^{-}]\left(\frac{\partial B}{\partial x_2} - \frac{\partial z}{\partial x_2}\right) \\ & + \frac{\gamma}{\alpha}\,[HCO_3^{-}]\,\frac{\partial[OH^{-}]}{\partial x_2}\end{aligned}$$

$$+ [OH^-][HCO_3^-]\left( \frac{1}{\alpha}\frac{\partial\gamma}{\partial x_2} - \frac{\gamma}{\alpha^2}\frac{\partial\alpha}{\partial x_2} \right)\Big\}$$

(A3-24)

(d) Using equation (A3-11) and equation (A3-13) with $x_1$ replaced by $x_2$:

$$\left(\frac{\partial f}{\partial x_2}\right)_z = (A-m+2B)\frac{\partial B}{\partial x_2} \qquad \text{(A3-25)}$$

and

$\left(\frac{\partial f}{\partial z}\right)_{x_2}$ is the same as in equation (A3-14)

(e) $$\left(\frac{\partial B}{\partial K_2}\right) = - P_T\, x_2\, H_2 \qquad \text{(A3-26)}$$

(f) Using equation (A3-11) and equation (A3-17) with $K_1$ replaced by $K_2$:

$$\left(\frac{\partial f}{\partial K_2}\right)_z = (A-m+2B)\frac{\partial B}{\partial K_2} \qquad \text{(A3-27)}$$

and

$\left(\frac{\partial f}{\partial z}\right)_{K_2}$ is the same as in equation (A3-18).

# APPENDIX 4

# COMPUTER PRINTOUTS FOR AMINE CONTACTOR AND REGENERATOR PROBLEMS

# APPENDIX 4.1 -- TEST PROBLEM 1 -- NASIR CORRELATION

```
     ***** PROBLEM STATEMENT *****


TYPE OF COLUMN          1

NO. OF PLATES        20

PRESSURE AT TOP PLATE (PSIA)              150.00

PRESSURE DROP PER PLATE (PSIA)               0.0

NO. OF FEEDS          3

       ENTERING PLATE OF FEED 1        1
       FEED QUANTITY        0.69583E+03
       PRESSURE OF FEED             150.00
       TEMPERATURE OF FEED (F)                100.00

       ENTERING PLATE OF FEED 2        4
       FEED QUANTITY        0.28612E+04
       PRESSURE OF FEED             150.00
       TEMPERATURE OF FEED (F)                120.00

       ENTERING PLATE OF FEED 3       20
       FEED QUANTITY        0.19686E+04
       PRESSURE OF FEED             150.00
       TEMPERATURE OF FEED (F)                 95.00
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.10760E+02
TEMPERATURE
 0.56960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
VAPOUR FLOW RATE
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04

 1   SUM OF SQUARES OF RESIDUALS  0.48618E-01
TEMPERATURE
 0.59037E+03 0.60638E+03 0.61723E+03 0.56538E+03 0.56538E+03
 0.56537E+03 0.56537E+03 0.56537E+03 0.56537E+03 0.56537E+03
 0.56537E+03 0.56537E+03 0.56537E+03 0.56536E+03 0.56533E+03
 0.56523E+03 0.56490E+03 0.56376E+03 0.55992E+03 0.54670E+03
VAPOUR FLOW RATE
 0.19656E+04 0.19768E+04 0.19830E+04 0.19533E+04 0.19532E+04
 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04
 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04
 0.19531E+04 0.19529E+04 0.19523E+04 0.19501E+04 0.19438E+04

 2   SUM OF SQUARES OF RESIDUALS  0.10229E-01
TEMPERATURE
 0.56636E+03 0.56294E+03 0.55723E+03 0.57477E+03 0.57477E+03
 0.57477E+03 0.57477E+03 0.57477E+03 0.57477E+03 0.57477E+03
 0.57477E+03 0.57476E+03 0.57475E+03 0.57471E+03 0.57461E+03
 0.57435E+03 0.57370E+03 0.57237E+03 0.57081E+03 0.57608E+03
VAPOUR FLOW RATE
 0.19506E+04 0.19365E+04 0.19149E+04 0.19592E+04 0.19590E+04
 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04
 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04
 0.19588E+04 0.19586E+04 0.19579E+04 0.19569E+04 0.19565E+04

 3   SUM OF SQUARES OF RESIDUALS  0.25122E-02
TEMPERATURE
 0.56618E+03 0.57807E+03 0.59692E+03 0.58306E+03 0.58306E+03
 0.58306E+03 0.58306E+03 0.58306E+03 0.58306E+03 0.58306E+03
 0.58306E+03 0.58305E+03 0.58304E+03 0.58301E+03 0.58294E+03
 0.58281E+03 0.58259E+03 0.58230E+03 0.58186E+03 0.57905E+03
VAPOUR FLOW RATE
 0.19549E+04 0.19593E+04 0.19644E+04 0.19643E+04 0.19642E+04
 0.19642E+04 0.19642E+04 0.19642E+04 0.19642E+04 0.19642E+04
 0.19642E+04 0.19642E+04 0.19641E+04 0.19641E+04 0.19641E+04
 0.19640E+04 0.19638E+04 0.19634E+04 0.19630E+04 0.19638E+04
 4   SUM OF SQUARES OF RESIDUALS  0.22373E-03
TEMPERATURE
 0.57459E+03 0.58010E+03 0.57874E+03 0.57949E+03 0.57949E+03
 0.57949E+03 0.57949E+03 0.57949E+03 0.57949E+03 0.57949E+03
 0.57949E+03 0.57948E+03 0.57947E+03 0.57943E+03 0.57937E+03
 0.57926E+03 0.57907E+03 0.57882E+03 0.57842E+03 0.57549E+03
VAPOUR FLOW RATE
 0.19583E+04 0.19618E+04 0.19585E+04 0.19630E+04 0.19628E+04
 0.19628E+04 0.19628E+04 0.19628E+04 0.19628E+04 0.19628E+04
 0.19628E+04 0.19628E+04 0.19628E+04 0.19628E+04 0.19628E+04
 0.19627E+04 0.19626E+04 0.19624E+04 0.19623E+04 0.19621E+04

 5   SUM OF SQUARES OF RESIDUALS  0.52480E-04
TEMPERATURE
 0.57064E+03 0.57502E+03 0.58019E+03 0.57984E+03 0.57984E+03
 0.57984E+03 0.57984E+03 0.57984E+03 0.57984E+03 0.57984E+03
 0.57984E+03 0.57983E+03 0.57982E+03 0.57980E+03 0.57977E+03
 0.57971E+03 0.57960E+03 0.57937E+03 0.57867E+03 0.57597E+03
VAPOUR FLOW RATE
 0.19567E+04 0.19589E+04 0.19620E+04 0.19631E+04 0.19629E+04
 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04
 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04
 0.19628E+04 0.19628E+04 0.19626E+04 0.19623E+04 0.19621E+04

 6   SUM OF SQUARES OF RESIDUALS  0.51550E-05
TEMPERATURE
 0.57177E+03 0.57817E+03 0.57988E+03 0.57978E+03 0.57978E+03
 0.57978E+03 0.57978E+03 0.57978E+03 0.57978E+03 0.57977E+03
 0.57977E+03 0.57977E+03 0.57976E+03 0.57975E+03 0.57972E+03
 0.57967E+03 0.57956E+03 0.57927E+03 0.57856E+03 0.57590E+03
VAPOUR FLOW RATE
 0.19573E+04 0.19607E+04 0.19619E+04 0.19631E+04 0.19629E+04
 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04
 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04 0.19629E+04
 0.19628E+04 0.19628E+04 0.19626E+04 0.19623E+04 0.19621E+04
```

```
     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS    6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.150E+03 PSIA    0.100E+03 F    0.290E+07 BTU     1.0

 0.150E+03 PSIA    0.120E+03 F    0.119E+08 BTU     1.0

 0.150E+03 PSIA    0.950E+02 F    0.128E+08 BTU     0.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP   LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F     LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1     150.00  112.17  0.69917E+03   0.19573E+04   0.0
  2     150.00  118.57  0.70036E+03   0.19607E+04   0.0
  3     150.00  120.28  0.70154E+03   0.19619E+04   0.0
  4     150.00  120.18  0.35626E+04   0.19631E+04   0.0
  5     150.00  120.18  0.35626E+04   0.19629E+04   0.0
  6     150.00  120.18  0.35626E+04   0.19629E+04   0.0
  7     150.00  120.18  0.35626E+04   0.19629E+04   0.0
  8     150.00  120.18  0.35626E+04   0.19629E+04   0.0
  9     150.00  120.18  0.35626E+04   0.19629E+04   0.0
 10     150.00  120.18  0.35626E+04   0.19629E+04   0.0
 11     150.00  120.17  0.35626E+04   0.19629E+04   0.0
 12     150.00  120.17  0.35626E+04   0.19629E+04   0.0
 13     150.00  120.16  0.35626E+04   0.19629E+04   0.0
 14     150.00  120.15  0.35625E+04   0.19629E+04   0.0
 15     150.00  120.12  0.35625E+04   0.19629E+04   0.0
 16     150.00  120.07  0.35624E+04   0.19628E+04   0.0
 17     150.00  119.96  0.35623E+04   0.19628E+04   0.0
 18     150.00  119.67  0.35619E+04   0.19626E+04   0.0
 19     150.00  118.96  0.35618E+04   0.19623E+04   0.0
 20     150.00  116.30  0.35683E+04   0.19621E+04   0.0
```

```
*** MATERIAL BALANCES ***

 FEEDS

                  PLATE NO.    1                       PLATE NO.    4
              LB MOL/TIME    MOL FRAC        LB MOL/TIME    MOL FRAC
 H2S          0.12800E+01   0.18395E-02     0.54300E+02   0.18978E-01
 CO2          0.15700E+01   0.22563E-02     0.63000E+01   0.22019E-02
 MEA          0.62050E+02   0.89174E-01     0.25000E+03   0.87377E-01
 WATER        0.63093E+03   0.90673E+00     0.25500E+04   0.89124E+00
 HYDROGEN     0.0           0.0             0.0           0.0
 NITROGEN     0.0           0.0             0.0           0.0
 METHANE      0.0           0.0             0.0           0.0
 ETHANE       0.0           0.0             0.16000E+00   0.55921E-04
 PROPANE      0.0           0.0             0.42000E+00   0.14679E-03
 N-BUTANE     0.0           0.0             0.0           0.0
 I-BUTANE     0.0           0.0             0.0           0.0
 TOTAL        0.69583E+03                   0.28612E+04

                  PLATE NO.   20                       PLATE NO.
              LB MOL/TIME    MOL FRAC        LB MOL/TIME    MOL FRAC
 H2S          0.18700E+02   0.94989E-02
 CO2          0.29500E+01   0.14985E-02
 MEA          0.0           0.0
 WATER        0.59100E+01   0.30021E-02
 HYDROGEN     0.62997E+03   0.32000E+00
 NITROGEN     0.29530E+02   0.15000E-01
 METHANE      0.78155E+03   0.39700E+00
 ETHANE       0.35436E+03   0.18000E+00
 PROPANE      0.12402E+03   0.62997E-01
 N-BUTANE     0.19700E+01   0.10007E-02
 I-BUTANE     0.19690E+02   0.10002E-01
 TOTAL        0.19686E+04

 PRODUCTS

                   TOP PRODUCT                      BOTTOM PRODUCT
              LB MOL/TIME    MOL FRAC        LB MOL/TIME    MOL FRAC
 H2S          0.19845E-01   0.10139E-04     0.74261E+02   0.20811E-01
 CO2          0.18589E-03   0.94969E-07     0.10820E+02   0.30322E-02
 MEA          0.38791E-01   0.19818E-04     0.31201E+03   0.87439E-01
 WATER        0.16185E+02   0.82690E-02     0.31707E+04   0.88856E+00
 HYDROGEN     0.62983E+03   0.32178E+00     0.16366E+00   0.45865E-04
 NITROGEN     0.29525E+02   0.15084E-01     0.54184E-02   0.15185E-05
 METHANE      0.78127E+03   0.39915E+00     0.26851E+00   0.75250E-04
 ETHANE       0.35443E+03   0.18108E+00     0.91760E-01   0.25715E-04
 PROPANE      0.12439E+03   0.63548E-01     0.35321E-01   0.98984E-05
 N-BUTANE     0.19699E+01   0.10064E-02     0.32667E-04   0.91548E-08
 I-BUTANE     0.19689E+02   0.10059E-01     0.32651E-03   0.91502E-07
 TOTAL        0.19573E+04                   0.35683E+04
```

# APPENDIX 4.2 -- TEST PROBLEM 2 -- NASIR CORRELATION

```
[illegible]* PROBLEM STATEMENT *****


TYPE OF COLUMN          1

NO. OF PLATES           4

PRESSURE AT TOP PLATE (PSIA)              712.00

PRESSURE DROP PER PLATE (PSIA)              0.0

NO. OF FEEDS          3

    ENTERING PLATE OF FEED 1          1
    FEED QUANTITY         0.75739E+05
    PRESSURE OF FEED               712.00
    TEMPERATURE OF FEED (F)                 135.00

    ENTERING PLATE OF FEED 2          2
    FEED QUANTITY         0.16323E+06
    PRESSURE OF FEED               712.00
    TEMPERATURE OF FEED (F)                 145.00

    ENTERING PLATE OF FEED 3          4
    FEED QUANTITY         0.28947E+05
    PRESSURE OF FEED               712.00
    TEMPERATURE OF FEED (F)                 100.00
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

  0   SUM OF SQUARES OF RESIDUALS  0.13961E+01
 TEMPERATURE
  0.59460E+03 0.59960E+03 0.60460E+03 0.60960E+03
 VAPOUR FLOW RATE
  0.21131E+05 0.21131E+05 0.21131E+05 0.21131E+05

  1   SUM OF SQUARES OF RESIDUALS  0.16383E-01
 TEMPERATURE
  0.59511E+03 0.58438E+03 0.58478E+03 0.58931E+03
 VAPOUR FLOW RATE
  0.21010E+05 0.21050E+05 0.21181E+05 0.21333E+05

  2   SUM OF SQUARES OF RESIDUALS  0.76640E-03
 TEMPERATURE
  0.59522E+03 0.60178E+03 0.60305E+03 0.62211E+03
 VAPOUR FLOW RATE
  0.21039E+05 0.21110E+05 0.21238E+05 0.21564E+05

  3   SUM OF SQUARES OF RESIDUALS  0.38484E-04
 TEMPERATURE
  0.59551E+03 0.60172E+03 0.60357E+03 0.62151E+03
 VAPOUR FLOW RATE
  0.21035E+05 0.21111E+05 0.21245E+05 0.21942E+05

  4   SUM OF SQUARES OF RESIDUALS  0.53383E-07
 TEMPERATURE
  0.59552E+03 0.60179E+03 0.60484E+03 0.62151E+03
 VAPOUR FLOW RATE
  0.21035E+05 0.21111E+05 0.21250E+05 0.21932E+05
```

```
     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS    4

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.712E+03 PSIA    0.135E+03 F    0.453E+09 BTU      1.0

 0.712E+03 PSIA    0.145E+03 F    0.924E+09 BTU      1.0

 0.712E+03 PSIA    0.100E+03 F    0.154E+09 BTU      0.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP   LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F     LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1     712.00  135.92  0.75816E+05   0.21035E+05   0.0
  2     712.00  142.19  0.23918E+06   0.21111E+05   0.0
  3     712.00  145.24  0.23986E+06   0.21250E+05   0.0
  4     712.00  161.91  0.24688E+06   0.21932E+05   0.0
```

```
*** MATERIAL BALANCES ***

 FEEDS

                 PLATE NO.    1                 PLATE NO.    2
             LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S         0.36300E+02  0.47928E-03    0.29050E+03  0.17797E-02
 CO2         0.28100E+02  0.37101E-03    0.14025E+03  0.85923E-03
 DEA         0.54150E+04  0.71495E-01    0.81475E+04  0.49915E-01
 WATER       0.70260E+05  0.92765E+00    0.15465E+06  0.94745E+00
 METHANE     0.0          0.0            0.0          0.0
 TOTAL       0.75739E+05                 0.16323E+06

                 PLATE NO.    4                 PLATE NO.
             LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S         0.69480E+04  0.24002E+00
 CO2         0.86840E+03  0.30000E-01
 DEA         0.0          0.0
 WATER       0.0          0.0
 METHANE     0.21131E+05  0.72998E+00
 TOTAL       0.28947E+05

 PRODUCTS

                   TOP PRODUCT                 BOTTOM PRODUCT
             LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S         0.66924E-01  0.31815E-05    0.72747E+04  0.29467E-01
 CO2         0.83405E-02  0.39650E-06    0.10367E+04  0.41994E-02
 DEA         0.52256E-03  0.24842E-07    0.13563E+05  0.54936E-01
 WATER       0.71579E+02  0.34028E-02    0.22484E+06  0.91072E+00
 METHANE     0.20964E+05  0.99659E+00    0.16680E+03  0.67562E-03
 TOTAL       0.21035E+05                 0.24688E+06
```

# APPENDIX 4.3 -- TEST PROBLEM 3 -- NASIR CORRELATION

```
     ***** PROBLEM STATEMENT *****


TYPE OF COLUMN        3

NO. OF PLATES       14

PRESSURE OF CONDENSER (PSIA)              27.00

PRESSURE AT TOP PLATE (PSIA)              28.00

PRESSURE DROP PER PLATE (PSIA)             0.3333

NO. OF FEEDS        1

    ENTERING PLATE OF FEED 1        2
    FEED QUANTITY         0.37194E+05
    PRESSURE OF FEED               100.00
    TEMPERATURE OF FEED (F)               200.00

NO. OF INTER COOLERS OR HEATERS           1

    PLATE NO. OF INTER COOLER OR HEATER 1       14
    HEAT LOAD OF INTER COOLER OR HEATER       0.11411E+09
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 * NEGATIVE PARTIAL PRESSURE(S) CALCULATED ARE
 H2S  0.238291E+01     CO2 -0.270499E-01

 * NEGATIVE PARTIAL PRESSURE(S) CALCULATED ARE
 H2S  0.254442E-01     CO2 -0.282249E-02

   0   SUM OF SQUARES OF RESIDUALS  0.73409E-01
  TEMPERATURE
   0.57960E+03 0.68960E+03 0.69960E+03 0.70160E+03 0.70360E+03
   0.70560E+03 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03
   0.71560E+03 0.71760E+03 0.71960E+03 0.72160E+03
  VAPOUR FLOW RATE
   0.11400E+04 0.34200E+04 0.50000E+04 0.51000E+04 0.52000E+04
   0.53000E+04 0.54000E+04 0.55000E+04 0.56000E+04 0.57000E+04
   0.58000E+04 0.59000E+04 0.60000E+04 0.61000E+04

   1   SUM OF SQUARES OF RESIDUALS  0.15207E-01
  TEMPERATURE
   0.57960E+03 0.68705E+03 0.69580E+03 0.70105E+03 0.70422E+03
   0.70621E+03 0.70757E+03 0.70895E+03 0.71226E+03 0.71401E+03
   0.71532E+03 0.71648E+03 0.71750E+03 0.71814E+03
  VAPOUR FLOW RATE
   0.10800E+04 0.28545E+04 0.46959E+04 0.51882E+04 0.54343E+04
   0.55555E+04 0.56241E+04 0.62446E+04 0.61653E+04 0.62659E+04
   0.63250E+04 0.64314E+04 0.66211E+04 0.68888E+04

   2   SUM OF SQUARES OF RESIDUALS  0.65676E-02
  TEMPERATURE
   0.57960E+03 0.69145E+03 0.69962E+03 0.70333E+03 0.70561E+03
   0.70726E+03 0.70855E+03 0.70961E+03 0.71197E+03 0.71349E+03
   0.71463E+03 0.71558E+03 0.71642E+03 0.71803E+03
  VAPOUR FLOW RATE
   0.11317E+04 0.35505E+04 0.50906E+04 0.55470E+04 0.57753E+04
   0.59341E+04 0.60839E+04 0.60150E+04 0.61885E+04 0.63430E+04
   0.64456E+04 0.65344E+04 0.66400E+04 0.67125E+04

   3   SUM OF SQUARES OF RESIDUALS  0.16778E-02
  TEMPERATURE
   0.57960E+03 0.68678E+03 0.69545E+03 0.70054E+03 0.70362E+03
   0.70567E+03 0.70747E+03 0.71067E+03 0.71246E+03 0.71373E+03
   0.71475E+03 0.71564E+03 0.71650E+03 0.71809E+03
  VAPOUR FLOW RATE
   0.11238E+04 0.29125E+04 0.45638E+04 0.51007E+04 0.54324E+04
   0.56340E+04 0.62236E+04 0.59381E+04 0.61748E+04 0.63117E+04
   0.64104E+04 0.64907E+04 0.65449E+04 0.65932E+04
 4   SUM OF SQUARES OF RESIDUALS  0.24386E-03
TEMPERATURE
 0.57960E+03 0.68940E+03 0.69760E+03 0.70205E+03 0.70478E+03
 0.70663E+03 0.70800E+03 0.71090E+03 0.71259E+03 0.71380E+03
 0.71479E+03 0.71568E+03 0.71653E+03 0.71809E+03
VAPOUR FLOW RATE
 0.11295E+04 0.33298E+04 0.49012E+04 0.53376E+04 0.55966E+04
 0.57781E+04 0.57800E+04 0.60276E+04 0.62240E+04 0.63453E+04
 0.64307E+04 0.64966E+04 0.65574E+04 0.66131E+04

 5   SUM OF SQUARES OF RESIDUALS  0.76442E-04
TEMPERATURE
 0.57960E+03 0.68743E+03 0.69582E+03 0.70077E+03 0.70382E+03
 0.70589E+03 0.70739E+03 0.71064E+03 0.71246E+03 0.71373E+03
 0.71475E+03 0.71566E+03 0.71652E+03 0.71808E+03
VAPOUR FLOW RATE
 0.11250E+04 0.31005E+04 0.46488E+04 0.51566E+04 0.54719E+04
 0.56564E+04 0.58512E+04 0.59855E+04 0.62083E+04 0.63346E+04
 0.64217E+04 0.64921E+04 0.65541E+04 0.66071E+04

 6   SUM OF SQUARES OF RESIDUALS  0.79214E-05
TEMPERATURE
 0.57960E+03 0.68842E+03 0.69666E+03 0.70133E+03 0.70421E+03
 0.70619E+03 0.70766E+03 0.71074E+03 0.71251E+03 0.71375E+03
 0.71477E+03 0.71566E+03 0.71652E+03 0.71808E+03
VAPOUR FLOW RATE
 0.11302E+04 0.32464E+04 0.48199E+04 0.52678E+04 0.55429E+04
 0.57375E+04 0.58466E+04 0.60085E+04 0.62193E+04 0.63422E+04
 0.64284E+04 0.64972E+04 0.65577E+04 0.66109E+04
```

```
    ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS    6

REFLUX RATIO          1.87243

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.100E+03 PSIA    0.200E+03 F    0.207E+09 BTU      1.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP    LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F      LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1      27.00  120.00   0.21162E+04   0.11302E+04 -0.41422E+08
  2      28.00  228.82   0.40884E+05   0.32464E+04  0.0
  3      28.33  237.06   0.41332E+05   0.48199E+04  0.0
  4      28.67  241.73   0.41607E+05   0.52678E+04  0.0
  5      29.00  244.61   0.41801E+05   0.55429E+04  0.0
  6      29.33  246.59   0.41910E+05   0.57375E+04  0.0
  7      29.67  248.06   0.42072E+05   0.58466E+04  0.0
  8      30.00  251.14   0.42283E+05   0.60085E+04  0.0
  9      30.33  252.91   0.42406E+05   0.62193E+04  0.0
 10      30.67  254.15   0.42492E+05   0.63422E+04  0.0
 11      31.00  255.17   0.42561E+05   0.64284E+04  0.0
 12      31.33  256.06   0.42621E+05   0.64972E+04  0.0
 13      31.67  256.92   0.42675E+05   0.65577E+04  0.0
 14      32.00  258.48   0.36064E+05   0.66109E+04  0.11411E+09
```

```
*** MATERIAL BALANCES ***

FEEDS

                 PLATE NO.    2                     PLATE NO.
           LB MOL/TIME    MOL FRAC        LB MOL/TIME    MOL FRAC
H2S        0.11402E+04    0.30656E-01
CO2        0.10180E+03    0.27370E-02
MEA        0.32200E+04    0.86573E-01
WATER      0.32730E+05    0.87998E+00
HYDROGEN   0.67000E+00    0.18014E-04
NITROGEN   0.40000E-01    0.10754E-05
METHANE    0.57000E+00    0.15325E-04
ETHANE     0.32000E+00    0.86036E-05
PROPANE    0.34000E+00    0.91413E-05
TOTAL      0.37194E+05

PRODUCTS

                 TOP PRODUCT                     BOTTOM PRODUCT
           LB MOL/TIME    MOL FRAC        LB MOL/TIME    MOL FRAC
H2S        0.10151E+04    0.89818E+00     0.12507E+03    0.34679E-02
CO2        0.42485E+02    0.37590E-01     0.59326E+02    0.16450E-02
MEA        0.12591E-01    0.11141E-04     0.32200E+04    0.89286E-01
WATER      0.70643E+02    0.62505E-01     0.32659E+05    0.90560E+00
HYDROGEN   0.66997E+00    0.59279E-03     0.24524E-30    0.68002E-35
NITROGEN   0.39998E-01    0.35390E-04     0.14811E-31    0.41069E-36
METHANE    0.56998E+00    0.50431E-03     0.20497E-30    0.56835E-35
ETHANE     0.31999E+00    0.28312E-03     0.11647E-30    0.32297E-35
PROPANE    0.33999E+00    0.30082E-03     0.12432E-30    0.34471E-35
TOTAL      0.11302E+04                    0.36064E+05
```

## APPENDIX 4.4 -- TEST PROBLEM 4 -- NASIR CORRELATION

```
     ***** PROBLEM STATEMENT *****


TYPE OF COLUMN        3

NO. OF PLATES      14

PRESSURE OF CONDENSER (PSIA)              25.00

PRESSURE AT TOP PLATE (PSIA)              27.00

PRESSURE DROP PER PLATE (PSIA)             0.3333

NO. OF FEEDS        1

   ENTERING PLATE OF FEED 1       2
   FEED QUANTITY         0.64652E+04
   PRESSURE OF FEED                48.00
   TEMPERATURE OF FEED (F)              180.00

NO. OF INTER COOLERS OR HEATERS          1

   PLATE NO. OF INTER COOLER OR HEATER 1       14
   HEAT LOAD OF INTER COOLER OR HEATER         0.16171E+08
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.13119E+01
TEMPERATURE
 0.55960E+03 0.67960E+03 0.69160E+03 0.69360E+03 0.69560E+03
 0.69760E+03 0.69960E+03 0.70160E+03 0.70360E+03 0.70560E+03
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03
VAPOUR FLOW RATE
 0.16000E+03 0.40000E+03 0.70000E+03 0.85000E+03 0.90000E+03
 0.90500E+03 0.91000E+03 0.91500E+03 0.92000E+03 0.92500E+03
 0.93000E+03 0.93500E+03 0.94000E+03 0.94500E+03

 1   SUM OF SQUARES OF RESIDUALS  0.60658E+00
TEMPERATURE
 0.55960E+03 0.68083E+03 0.70406E+03 0.71532E+03 0.71772E+03
 0.71510E+03 0.71142E+03 0.70892E+03 0.70802E+03 0.70846E+03
 0.70929E+03 0.71061E+03 0.71219E+03 0.71382E+03
VAPOUR FLOW RATE
 0.15811E+03 0.40919E+03 0.11628E+04 0.17000E+04 0.17940E+04
 0.15993E+04 0.13649E+04 0.11829E+04 0.10692E+04 0.10334E+04
 0.97892E+03 0.95271E+03 0.95045E+03 0.96213E+03

 2   SUM OF SQUARES OF RESIDUALS  0.40929E-01
TEMPERATURE
 0.55960E+03 0.68274E+03 0.70159E+03 0.71046E+03 0.71284E+03
 0.71108E+03 0.70955E+03 0.70954E+03 0.71032E+03 0.71106E+03
 0.71181E+03 0.71262E+03 0.71348E+03 0.71433E+03
VAPOUR FLOW RATE
 0.14895E+03 0.41116E+03 0.79477E+03 0.85000E+03 0.93640E+03
 0.10469E+04 0.11254E+04 0.11478E+04 0.11187E+04 0.10569E+04
 0.99671E+03 0.96144E+03 0.96219E+03 0.98713E+03

 3   SUM OF SQUARES OF RESIDUALS  0.30413E-01
TEMPERATURE
 0.55960E+03 0.67193E+03 0.69525E+03 0.70264E+03 0.70619E+03
 0.70738E+03 0.70826E+03 0.70920E+03 0.71010E+03 0.71091E+03
 0.71169E+03 0.71244E+03 0.71313E+03 0.71417E+03
VAPOUR FLOW RATE
 0.15120E+03 0.25868E+03 0.60126E+03 0.79191E+03 0.85373E+03
 0.90686E+03 0.93104E+03 0.93041E+03 0.92620E+03 0.93081E+03
 0.93116E+03 0.93446E+03 0.94412E+03 0.95226E+03
 4   SUM OF SQUARES OF RESIDUALS  0.11390E-01
TEMPERATURE
 0.55960E+03 0.69421E+03 0.70902E+03 0.70736E+03 0.70743E+03
 0.70822E+03 0.70893E+03 0.70967E+03 0.71041E+03 0.71112E+03
 0.71181E+03 0.71248E+03 0.71316E+03 0.71422E+03
VAPOUR FLOW RATE
 0.15218E+03 0.43760E+03 0.10779E+04 0.10142E+04 0.10206E+04
 0.94482E+03 0.91686E+03 0.91574E+03 0.91948E+03 0.92328E+03
 0.92856E+03 0.93587E+03 0.94158E+03 0.94372E+03

 5   SUM OF SQUARES OF RESIDUALS  0.10163E-01
TEMPERATURE
 0.55960E+03 0.68785E+03 0.70613E+03 0.70605E+03 0.70694E+03
 0.70783E+03 0.70862E+03 0.70941E+03 0.71017E+03 0.71091E+03
 0.71162E+03 0.71232E+03 0.71304E+03 0.71416E+03
VAPOUR FLOW RATE
 0.14345E+03 0.32820E+03 0.83056E+03 0.93827E+03 0.94255E+03
 0.91527E+03 0.90542E+03 0.90866E+03 0.91426E+03 0.91987E+03
 0.92618E+03 0.93307E+03 0.93886E+03 0.94314E+03

 6   SUM OF SQUARES OF RESIDUALS  0.49111E-02
TEMPERATURE
 0.55960E+03 0.68023E+03 0.70188E+03 0.70433E+03 0.70624E+03
 0.70746E+03 0.70843E+03 0.70930E+03 0.71009E+03 0.71086E+03
 0.71160E+03 0.71232E+03 0.71305E+03 0.71416E+03
VAPOUR FLOW RATE
 0.14794E+03 0.30456E+03 0.69042E+03 0.90918E+03 0.92668E+03
 0.92673E+03 0.92603E+03 0.92887E+03 0.93509E+03 0.94009E+03
 0.94510E+03 0.94930E+03 0.95216E+03 0.95401E+03

 7   SUM OF SQUARES OF RESIDUALS  0.63528E-03
TEMPERATURE
 0.55960E+03 0.67499E+03 0.69641E+03 0.70291E+03 0.70588E+03
 0.70735E+03 0.70841E+03 0.70929E+03 0.71010E+03 0.71087E+03
 0.71161E+03 0.71234E+03 0.71306E+03 0.71416E+03
VAPOUR FLOW RATE
 0.15119E+03 0.33342E+03 0.64897E+03 0.87725E+03 0.90757E+03
 0.92076E+03 0.92451E+03 0.92883E+03 0.93164E+03 0.93576E+03
 0.93979E+03 0.94338E+03 0.94667E+03 0.94931E+03
 8   SUM OF SQUARES OF RESIDUALS  0.10255E-03
TEMPERATURE
 0.55960E+03 0.67626E+03 0.69710E+03 0.70315E+03 0.70600E+03
 0.70744E+03 0.70848E+03 0.70935E+03 0.71015E+03 0.71091E+03
 0.71164E+03 0.71237E+03 0.71308E+03 0.71418E+03
VAPOUR FLOW RATE
 0.14975E+03 0.33970E+03 0.69809E+03 0.87492E+03 0.89789E+03
 0.90970E+03 0.91465E+03 0.91937E+03 0.92362E+03 0.92841E+03
 0.93315E+03 0.93773E+03 0.94222E+03 0.94605E+03

 9   SUM OF SQUARES OF RESIDUALS  0.18993E-04
TEMPERATURE
 0.55960E+03 0.67806E+03 0.69781E+03 0.70341E+03 0.70612E+03
 0.70752E+03 0.70853E+03 0.70939E+03 0.71017E+03 0.71092E+03
 0.71165E+03 0.71236E+03 0.71307E+03 0.71416E+03
VAPOUR FLOW RATE
 0.14807E+03 0.35130E+03 0.73334E+03 0.87051E+03 0.89044E+03
 0.90239E+03 0.90875E+03 0.91414E+03 0.91962E+03 0.92497E+03
 0.93048E+03 0.93593E+03 0.94112E+03 0.94581E+03

10   SUM OF SQUARES OF RESIDUALS  0.62679E-05
TEMPERATURE
 0.55960E+03 0.67745E+03 0.69751E+03 0.70331E+03 0.70607E+03
 0.70748E+03 0.70849E+03 0.70935E+03 0.71013E+03 0.71088E+03
 0.71160E+03 0.71232E+03 0.71304E+03 0.71415E+03
VAPOUR FLOW RATE
 0.14794E+03 0.34532E+03 0.71843E+03 0.86818E+03 0.89197E+03
 0.90486E+03 0.91128E+03 0.91685E+03 0.92227E+03 0.92776E+03
 0.93315E+03 0.93834E+03 0.94315E+03 0.94720E+03
```

```
     ***** COMPUTED RESULTS *****

   NUMBER OF ITERATIONS   10

   REFLUX RATIO            1.33415

   PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

    0.480E+02 PSIA    0.180E+03 F    0.373E+08 BTU     1.0

   *** STAGE VARIABLES ***

   PLATE  PRESSURE  TEMP    LIQUID FLOW    VAPOUR FLOW    HEAT DUTY
    NO.     PSIA     F      LB MOL/TIME    LB MOL/TIME    BTU/TIME
     1     25.00   100.00   0.19738E+03    0.14794E+03   -0.25199E+07
     2     27.00   217.85   0.70357E+04    0.34532E+03    0.0
     3     27.33   237.91   0.71855E+04    0.71843[illegible]    0.0
     4     27.67   243.71   0.72093E+04    0.86818E+03    0.0
     5     28.00   246.47   0.72221E+04    0.89197E+03    0.0
     6     28.33   247.88   0.72286E+04    0.90486E+03    0.0
     7     28.67   248.89   0.72341E+04    0.91128E+03    0.0
     8     29.00   249.75   0.72395E+04    0.91685E+03    0.0
     9     29.33   250.53   0.72450E+04    0.92227E+03    0.0
    10     29.67   251.28   0.72504E+04    0.92776E+03    0.0
    11     30.00   252.00   0.72556E+04    0.93315E+03    0.0
    12     30.33   252.72   0.72604E+04    0.93834E+03    0.0
    13     30.67   253.44   0.72645E+04    0.94315E+03    0.0
    14     31.00   254.55   0.63173E+04    0.94720E+03    0.16171E+08
```

```
*** MATERIAL BALANCES ***

FEEDS

               PLATE NO.    2                  PLATE NO.
            LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
H2S         0.37820E+02  0.58498E-02
CO2         0.12371E+03  0.19135E-01
DEA         0.29088E+03  0.44991E-01
WATER       0.60124E+04  0.92995E+00
METHANE     0.43000E+00  0.66510E-04
ETHANE      0.30000E-01  0.46402E-05
PROPANE     0.10000E-01  0.15467E-05
TOTAL       0.64652E+04

PRODUCTS

                TOP PRODUCT                   BOTTOM PRODUCT
            LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
H2S         0.35121E+02  0.23739E+00   0.26943E+01  0.42649E-03
CO2         0.10672E+03  0.72138E+00   0.16976E+02  0.26872E-02
DEA         0.49738E-08  0.33619E-10   0.29088E+03  0.46045E-01
WATER       0.56298E+01  0.38054E-01   0.60067E+04  0.95084E+00
METHANE     0.42992E+00  0.29060E-02   0.11638E-27  0.18423E-31
ETHANE      0.29995E-01  0.20274E-03   0.84490E-29  0.13375E-32
PROPANE     0.99982E-02  0.67581E-04   0.28948E-29  0.45824E-33
TOTAL       0.14794E+03                0.63173E+04
```

# APPENDIX 4.5 -- TEST PROBLEM 1 -- AMOCO CORRELATION

```
    ***** PROBLEM STATEMENT *****


TYPE OF COLUMN        1

NO. OF PLATES     20

PRESSURE AT TOP PLATE (PSIA)           150.00

PRESSURE DROP PER PLATE (PSIA)           0.0

NO. OF FEEDS      3

   ENTERING PLATE OF FEED 1       1
   FEED QUANTITY       0.69583E+03
   PRESSURE OF FEED          150.00
   TEMPERATURE OF FEED (F)          100.00

   ENTERING PLATE OF FEED 2       4
   FEED QUANTITY       0.28612E+04
   PRESSURE OF FEED          150.00
   TEMPERATURE OF FEED (F)          120.00

   ENTERING PLATE OF FEED 3      20
   FEED QUANTITY       0.19686E+04
   PRESSURE OF FEED          150.00
   TEMPERATURE OF FEED (F)           95.00
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

  0   SUM OF SQUARES OF RESIDUALS  0.10761E+02
 TEMPERATURE
  0.56960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
  0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
  0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
  0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
 VAPOUR FLOW RATE
  0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
  0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
  0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
  0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04

  1   SUM OF SQUARES OF RESIDUALS  0.48449E-01
 TEMPERATURE
  0.59020E+03 0.60612E+03 0.61692E+03 0.56531E+03 0.56531E+03
  0.56531E+03 0.56531E+03 0.56531E+03 0.56531E+03 0.56531E+03
  0.56531E+03 0.56531E+03 0.56531E+03 0.56530E+03 0.56527E+03
  0.56517E+03 0.56484E+03 0.56371E+03 0.55989E+03 0.54677E+03
 VAPOUR FLOW RATE
  0.19654E+04 0.19765E+04 0.19826E+04 0.19533E+04 0.19532E+04
  0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04
  0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04 0.19532E+04
  0.19531E+04 0.19529E+04 0.19523E+04 0.19501E+04 0.19433E+04

  2   SUM OF SQUARES OF RESIDUALS  0.10473E-01
 TEMPERATURE
  0.56619E+03 0.56268E+03 0.55692E+03 0.57490E+03 0.57490E+03
  0.57490E+03 0.57490E+03 0.57490E+03 0.57490E+03 0.57490E+03
  0.57490E+03 0.57490E+03 0.57488E+03 0.57485E+03 0.57474E+03
  0.57448E+03 0.57382E+03 0.57247E+03 0.57080E+03 0.57636E+03
 VAPOUR FLOW RATE
  0.19505E+04 0.19364E+04 0.19151E+04 0.19598E+04 0.19597E+04
  0.19597E+04 0.19597E+04 0.19597E+04 0.19597E+04 0.19597E+04
  0.19597E+04 0.19597E+04 0.19596E+04 0.19596E+04 0.19596E+04
  0.19595E+04 0.19591E+04 0.19585E+04 0.19574E+04 0.19580E+04

  3   SUM OF SQUARES OF RESIDUALS  0.26886E-02
 TEMPERATURE
  0.56663E+03 0.57893E+03 0.59804E+03 0.58326E+03 0.58326E+03
  0.58326E+03 0.58326E+03 0.58326E+03 0.58325E+03 0.58325E+03
  0.58325E+03 0.58325E+03 0.58323E+03 0.58320E+03 0.58313E+03
  0.58299E+03 0.58278E+03 0.58254E+03 0.58223E+03 0.57896E+03
 VAPOUR FLOW RATE
  0.19550E+04 0.19595E+04 0.19646E+04 0.19651E+04 0.19649E+04
  0.19649E+04 0.19649E+04 0.19649E+04 0.19649E+04 0.19649E+04
  0.19649E+04 0.19649E+04 0.19649E+04 0.19649E+04 0.19649E+04
  0.19647E+04 0.19645E+04 0.19643E+04 0.19639E+04 0.19642E+04
 4   SUM OF SQUARES OF RESIDUALS  0.23405E-03
TEMPERATURE
 0.57491E+03 0.58062E+03 0.57964E+03 0.57965E+03 0.57965E+03
 0.57965E+03 0.57965E+03 0.57965E+03 0.57964E+03 0.57964E+03
 0.57964E+03 0.57963E+03 0.57962E+03 0.57959E+03 0.57952E+03
 0.57941E+03 0.57923E+03 0.57895E+03 0.57838E+03 0.57536E+03
VAPOUR FLOW RATE
 0.19584E+04 0.19620E+04 0.19586E+04 0.19631E+04 0.19630E+04
 0.19630E+04 0.19630E+04 0.19630E+04 0.19630E+04 0.19630E+04
 0.19630E+04 0.19630E+04 0.19630E+04 0.19630E+04 0.19629E+04
 0.19628E+04 0.19627E+04 0.19626E+04 0.19623E+04 0.19618E+04

 5   SUM OF SQUARES OF RESIDUALS  0.56894E-04
TEMPERATURE
 0.57067E+03 0.57499E+03 0.58037E+03 0.57988E+03 0.57988E+03
 0.57988E+03 0.57988E+03 0.57988E+03 0.57987E+03 0.57987E+03
 0.57987E+03 0.57986E+03 0.57985E+03 0.57983E+03 0.57980E+03
 0.57973E+03 0.57960E+03 0.57931E+03 0.57856E+03 0.57594E+03
VAPOUR FLOW RATE
 0.19566E+04 0.19587E+04 0.19620E+04 0.19634E+04 0.19632E+04
 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04
 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04
 0.19632E+04 0.19631E+04 0.19629E+04 0.19625E+04 0.19623E+04

 6   SUM OF SQUARES OF RESIDUALS  0.60179E-05
TEMPERATURE
 0.57199E+03 0.57860E+03 0.58037E+03 0.57987E+03 0.57987E+03
 0.57987E+03 0.57987E+03 0.57987E+03 0.57986E+03 0.57986E+03
 0.57986E+03 0.57986E+03 0.57985E+03 0.57984E+03 0.57981E+03
 0.57975E+03 0.57962E+03 0.57931E+03 0.57857E+03 0.57586E+03
VAPOUR FLOW RATE
 0.19574E+04 0.19608E+04 0.19620E+04 0.19634E+04 0.19632E+04
 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04
 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04 0.19632E+04
 0.19632E+04 0.19631E+04 0.19629E+04 0.19625E+04 0.19623E+04
```

```
    ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS   6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.150E+03 PSIA    0.100E+03 F    0.290E+07 BTU     1.0

 0.150E+03 PSIA    0.120E+03 F    0.119E+08 BTU     1.0

 0.150E+03 PSIA    0.950E+02 F    0.128E+08 BTU     0.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP   LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F     LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1     150.00  112.39  0.69927E+03   0.19574E+04   0.0
  2     150.00  119.00  0.70047E+03   0.19608E+04   0.0
  3     150.00  120.77  0.70185E+03   0.19620E+04   0.0
  4     150.00  120.27  0.35629E+04   0.19634E+04   0.0
  5     150.00  120.27  0.35629E+04   0.19632E+04   0.0
  6     150.00  120.27  0.35629E+04   0.19632E+04   0.0
  7     150.00  120.27  0.35629E+04   0.19632E+04   0.0
  8     150.00  120.27  0.35629E+04   0.19632E+04   0.0
  9     150.00  120.27  0.35629E+04   0.19632E+04   0.0
 10     150.00  120.26  0.35629E+04   0.19632E+04   0.0
 11     150.00  120.26  0.35629E+04   0.19632E+04   0.0
 12     150.00  120.26  0.35629E+04   0.19632E+04   0.0
 13     150.00  120.25  0.35629E+04   0.19632E+04   0.0
 14     150.00  120.24  0.35629E+04   0.19632E+04   0.0
 15     150.00  120.21  0.35628E+04   0.19632E+04   0.0
 16     150.00  120.15  0.35627E+04   0.19632E+04   0.0
 17     150.00  120.02  0.35625E+04   0.19631E+04   0.0
 18     150.00  119.72  0.35622E+04   0.19629E+04   0.0
 19     150.00  118.97  0.35619E+04   0.19625E+04   0.0
 20     150.00  116.26  0.35683E+04   0.19623E+04   0.0
```

```
*** MATERIAL BALANCES ***

 FEEDS

               PLATE NO.    1                 PLATE NO.    4
           LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S       0.12800E+01   0.18395E-02   0.54300E+02   0.18978E-01
 CO2       0.15700E+01   0.22563E-02   0.63000E+01   0.22019E-02
 MEA       0.62050E+02   0.89174E-01   0.25000E+03   0.87377E-01
 H2O       0.63093E+03   0.90673E+00   0.25500E+04   0.89124E+00
 HYDROGEN  0.0           0.0           0.0           0.0
 NITROGEN  0.0           0.0           0.0           0.0
 METHANE   0.0           0.0           0.0           0.0
 ETHANE    0.0           0.0           0.16000E+00   0.55921E-04
 PROPANE   0.0           0.0           0.42000E+00   0.14679E-03
 NBUTANE   0.0           0.0           0.0           0.0
 IBUTANE   0.0           0.0           0.0           0.0
 TOTAL     0.69583E+03                 0.28612E+04

               PLATE NO.   20                 PLATE NO.
           LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S       0.18700E+02   0.94989E-02
 CO2       0.29500E+01   0.14985E-02
 MEA       0.0           0.0
 H2O       0.59100E+01   0.30021E-02
 HYDROGEN  0.62997E+03   0.32000E+00
 NITROGEN  0.29530E+02   0.15000E-01
 METHANE   0.78155E+03   0.39700E+00
 ETHANE    0.35436E+03   0.18000E+00
 PROPANE   0.12402E+03   0.62997E-01
 NBUTANE   0.19700E+01   0.10007E-02
 IBUTANE   0.19690E+02   0.10002E-01
 TOTAL     0.19686E+04

 PRODUCTS

                 TOP PRODUCT                BOTTOM PRODUCT
           LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S       0.30962E-01   0.15818E-04   0.74249E+02   0.20808E-01
 CO2       0.42326E-03   0.21624E-06   0.10820E+02   0.30321E-02
 MEA       0.38818E-01   0.19832E-04   0.31201E+03   0.87439E-01
 H2O       0.16195E+02   0.82738E-02   0.31707E+04   0.88856E+00
 HYDROGEN  0.62984E+03   0.32178E+00   0.16365E+00   0.45862E-04
 NITROGEN  0.29525E+02   0.15084E-01   0.54187E-02   0.15186E-05
 METHANE   0.78126E+03   0.39914E+00   0.26857E+00   0.75264E-04
 ETHANE    0.35443E+03   0.18108E+00   0.91769E-01   0.25718E-04
 PROPANE   0.12438E+03   0.63544E-01   0.35337E-01   0.99030E-05
 NBUTANE   0.19699E+01   0.10064E-02   0.32656E-04   0.91517E-08
 IBUTANE   0.19689E+02   0.10059E-01   0.32640E-03   0.91471E-07
 TOTAL     0.19574E+04                 0.35683E+04
```

# APPENDIX 4.6 -- TEST PROBLEM 2 -- AMOCO CORRELATION

```
    ***** PROBLEM STATEMENT *****


TYPE OF COLUMN       1

NO. OF PLATES       4

PRESSURE AT TOP PLATE (PSIA)             712.00

PRESSURE DROP PER PLATE (PSIA)             0.0

NO. OF FEEDS       3

    ENTERING PLATE OF FEED 1        1
    FEED QUANTITY         0.75739E+05
    PRESSURE OF FEED              712.00
    TEMPERATURE OF FEED (F)                 135.00

    ENTERING PLATE OF FEED 2        2
    FEED QUANTITY         0.16323E+06
    PRESSURE OF FEED              712.00
    TEMPERATURE OF FEED (F)                 145.00

    ENTERING PLATE OF FEED 3        4
    FEED QUANTITY         0.28947E+05
    PRESSURE OF FEED              712.00
    TEMPERATURE OF FEED (F)                 100.00
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.13973E+01
TEMPERATURE
 0.59460E+03 0.59960E+03 0.60460E+03 0.60960E+03
VAPOUR FLOW RATE
 0.21131E+05 0.21131E+05 0.21131E+05 0.21131E+05

 1   SUM OF SQUARES OF RESIDUALS  0.16778E-01
TEMPERATURE
 0.59510E+03 0.58437E+03 0.58478E+03 0.58931E+03
VAPOUR FLOW RATE
 0.21010E+05 0.21049E+05 0.21180E+05 0.21235E+05

 2   SUM OF SQUARES OF RESIDUALS  0.17026E-02
TEMPERATURE
 0.59522E+03 0.60177E+03 0.60273E+03 0.62211E+03
VAPOUR FLOW RATE
 0.21039E+05 0.21110E+05 0.21238E+05 0.21613E+05

 3   SUM OF SQUARES OF RESIDUALS  0.10453E-05
TEMPERATURE
 0.59551E+03 0.60173E+03 0.60379E+03 0.62151E+03
VAPOUR FLOW RATE
 0.21033E+05 0.21109E+05 0.21241E+05 0.21690E+05
```

```
    ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS    3

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.712E+03 PSIA    0.135E+03 F    0.453E+09 BTU      1.0

 0.712E+03 PSIA    0.145E+03 F    0.924E+09 BTU      1.0

 0.712E+03 PSIA    0.100E+03 F    0.154E+09 BTU      0.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP    LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F      LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1     712.00  135.91   0.75816E+05   0.21033E+05   0.0
  2     712.00  142.13   0.23918E+06   0.21109E+05   0.0
  3     712.00  144.19   0.23963E+06   0.21241E+05   0.0
  4     712.00  161.91   0.24688E+06   0.21690E+05   0.0
```

```
*** MATERIAL BALANCES ***

 FEEDS

                  PLATE NO.    1                     PLATE NO.    2
             LB MOL/TIME   MOL FRAC         LB MOL/TIME   MOL FRAC
 H2S         0.36300E+02  0.47928E-03      0.29050E+03  0.17797E-02
 CO2         0.28100E+02  0.37101E-03      0.14025E+03  0.85923E-03
 DEA         0.54150E+04  0.71495E-01      0.81475E+04  0.49915E-01
 H2O         0.70260E+05  0.92765E+00      0.15465E+06  0.94745E+00
 METHANE     0.0          0.0              0.0          0.0
 TOTAL       0.75739E+05                   0.16323E+06

                  PLATE NO.    4                     PLATE NO.
             LB MOL/TIME   MOL FRAC         LB MOL/TIME   MOL FRAC
 H2S         0.69480E+04  0.24002E+00
 CO2         0.86840E+03  0.30000E-01
 DEA         0.0          0.0
 H2O         0.0          0.0
 METHANE     0.21131E+05  0.72998E+00
 TOTAL       0.28947E+05

 PRODUCTS

                    TOP PRODUCT                      BOTTOM PRODUCT
             LB MOL/TIME   MOL FRAC         LB MOL/TIME   MOL FRAC
 H2S         0.33056E-01  0.15716E-05      0.72748E+04  0.29467E-01
 CO2         0.20321E-02  0.96614E-07      0.10367E+04  0.41994E-02
 DEA         0.52450E-03  0.24937E-07      0.13563E+05  0.54935E-01
 H2O         0.71196E+02  0.33850E-02      0.22484E+06  0.91072E+00
 METHANE     0.20962E+05  0.99661E+00      0.16870E+03  0.68332E-03
 TOTAL       0.21033E+05                   0.24688E+06
```

# APPENDIX 4.7 -- TEST PROBLEM 3 -- AMOCO CORRELATION

```
    ***** PROBLEM STATEMENT *****


TYPE OF COLUMN       3

NO. OF PLATES      14

PRESSURE OF CONDENSER (PSIA)            27.00

PRESSURE AT TOP PLATE (PSIA)            28.00

PRESSURE DROP PER PLATE (PSIA)          0.3333

NO. OF FEEDS       1

    ENTERING PLATE OF FEED 1       2
    FEED QUANTITY       0.37194E+05
    PRESSURE OF FEED           100.00
    TEMPERATURE OF FEED (F)          200.00

NO. OF INTER COOLERS OR HEATERS       1

    PLATE NO. OF INTER COOLER OR HEATER 1      14
    HEAT LOAD OF INTER COOLER OR HEATER       0.11411E+09
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.26205E+00
TEMPERATURE
 0.57960E+03 0.68960E+03 0.69960E+03 0.70160E+03 0.70360E+03
 0.70560E+03 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03
 0.71560E+03 0.71760E+03 0.71960E+03 0.72160E+03
VAPOUR FLOW RATE
 0.11400E+04 0.34200E+04 0.50000E+04 0.51000E+04 0.52000E+04
 0.53000E+04 0.54000E+04 0.55000E+04 0.56000E+04 0.57000E+04
 0.58000E+04 0.59000E+04 0.60000E+04 0.61000E+04

 1   SUM OF SQUARES OF RESIDUALS  0.37847E-01
TEMPERATURE
 0.57960E+03 0.68950E+03 0.70042E+03 0.70641E+03 0.70980E+03
 0.71151E+03 0.71240E+03 0.71303E+03 0.71368E+03 0.71444E+03
 0.71532E+03 0.71627E+03 0.71723E+03 0.71801E+03
VAPOUR FLOW RATE
 0.10779E+04 0.31658E+04 0.56570E+04 0.63350E+04 0.65563E+04
 0.65797E+04 0.65053E+04 0.64120E+04 0.63447E+04 0.63257E+04
 0.63654E+04 0.64685E+04 0.66388E+04 0.68862E+04

 2   SUM OF SQUARES OF RESIDUALS  0.89532E-03
TEMPERATURE
 0.57960E+03 0.69033E+03 0.70034E+03 0.70531E+03 0.70815E+03
 0.70990E+03 0.71115E+03 0.71217E+03 0.71309E+03 0.71396E+03
 0.71481E+03 0.71565E+03 0.71651E+03 0.71815E+03
VAPOUR FLOW RATE
 0.11328E+04 0.35037E+04 0.50716E+04 0.55503E+04 0.58848E+04
 0.61111E+04 0.62559E+04 0.63459E+04 0.64048E+04 0.64498E+04
 0.64927E+04 0.65428E+04 0.66162E+04 0.66775E+04

 3   SUM OF SQUARES OF RESIDUALS  0.13085E-03
TEMPERATURE
 0.57960E+03 0.68717E+03 0.69784E+03 0.70375E+03 0.70706E+03
 0.70916E+03 0.71067E+03 0.71189E+03 0.71294E+03 0.71389E+03
 0.71479E+03 0.71565E+03 0.71652E+03 0.71814E+03
VAPOUR FLOW RATE
 0.11318E+04 0.30258E+04 0.46829E+04 0.53552E+04 0.57438E+04
 0.59709E+04 0.61153E+04 0.62168E+04 0.62956E+04 0.63626E+04
 0.64239E+04 0.64829E+04 0.65409E+04 0.66001E+04
 4   SUM OF SQUARES OF RESIDUALS  0.15814E-04
TEMPERATURE
 0.57960E+03 0.68870E+03 0.69870E+03 0.70420E+03 0.70731E+03
 0.70931E+03 0.71077E+03 0.71195E+03 0.71298E+03 0.71393E+03
 0.71482E+03 0.71568E+03 0.71655E+03 0.71815E+03
VAPOUR FLOW RATE
 0.11429E+04 0.32854E+04 0.48778E+04 0.54393E+04 0.57769E+04
 0.59785E+04 0.61118E+04 0.62108E+04 0.62912E+04 0.63608E+04
 0.64239E+04 0.64833E+04 0.65419E+04 0.65983E+04

 5   SUM OF SQUARES OF RESIDUALS  0.39864E-05
TEMPERATURE
 0.57960E+03 0.68781E+03 0.69806E+03 0.70387E+03 0.70714E+03
 0.70921E+03 0.71071E+03 0.71191E+03 0.71295E+03 0.71390E+03
 0.71479E+03 0.71566E+03 0.71653E+03 0.71814E+03
VAPOUR FLOW RATE
 0.11360E+04 0.31703E+04 0.47453E+04 0.53621E+04 0.57343E+04
 0.59538E+04 0.60956E+04 0.61983E+04 0.62805E+04 0.63512E+04
 0.64154E+04 0.64765E+04 0.65366E+04 0.65942E+04
```

```
     ***** COMPUTED RESULTS *****

 NUMBER OF ITERATIONS = 5 .

 REFLUX RATIO          1.79074

 PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

  0.100E+03 PSIA    0.200E+03 F    0.207E+09 BTU     1.0

 *** STAGE VARIABLES ***

 PLATE  PRESSURE   TEMP    LIQUID FLOW    VAPOUR FLOW   HEAT DUTY
  NO.     PSIA      F      LB MOL/TIME    LB MOL/TIME   BTU/TIME
   1      27.00   120.00   0.20343E+04    0.11360E+04  -0.41285E+08
   2      28.00   228.21   0.40803E+05    0.31703E+04   0.0
   3      28.33   238.46   0.41420E+05    0.47453E+04   0.0
   4      28.67   244.27   0.41792E+05    0.53621E+04   0.0
   5      29.00   247.54   0.42012E+05    0.57343E+04   0.0
   6      29.33   249.61   0.42154E+05    0.59538E+04   0.0
   7      29.67   251.11   0.42256E+05    0.60956E+04   0.0
   8      30.00   252.31   0.42338E+05    0.61983E+04   0.0
   9      30.33   253.35   0.42409E+05    0.62805E+04   0.0
  10      30.67   254.30   0.42473E+05    0.63512E+04   0.0
  11      31.00   255.19   0.42534E+05    0.64154E+04   0.0
  12      31.33   256.06   0.42595E+05    0.64765E+04   0.0
  13      31.67   256.93   0.42652E+05    0.65366E+04   0.0
  14      32.00   258.54   0.36058E+05    0.65942E+04   0.11411E+09
```

```
*** MATERIAL BALANCES ***

FEEDS

                PLATE NO.   2                  PLATE NO.
           LB MOL/TIME    MOL FRAC      LB MOL/TIME    MOL FRAC
H2S        0.11402E+04   0.30656E-01
CO2        0.10180E+03   0.27370E-02
MEA        0.32200E+04   0.86573E-01
H2O        0.32730E+05   0.87998E+00
HYDROGEN   0.67000E+00   0.18014E-04
NITROGEN   0.40000E-01   0.10754E-05
METHANE    0.57000E+00   0.15325E-04
ETHANE     0.32000E+00   0.86036E-05
PROPANE    0.34000E+00   0.91413E-05
TOTAL      0.37194E+05

PRODUCTS

                  TOP PRODUCT                  BOTTOM PRODUCT
           LB MOL/TIME    MOL FRAC.     LB MOL/TIME    MOL FRAC
H2S        0.10460E+04   0.92073E+00   0.94226E+02   0.26132E-02
CO2        0.17478E+02   0.15385E-01   0.84338E+02   0.23389E-02
MEA        0.12464E-01   0.10972E-04   0.32200E+04   0.89300E-01
H2O        0.70616E+02   0.62162E-01   0.32659E+05   0.90575E+00
HYDROGEN   0.66999E+00   0.58978E-03   0.36649E-28   0.10164E-32
NITROGEN   0.39999E-01   0.35211E-04   0.20464E-29   0.56753E-34
METHANE    0.56999E+00   0.50175E-03   0.33366E-28   0.92535E-33
ETHANE     0.31999E+00   0.28168E-03   0.18012E-28   0.49954E-33
PROPANE    0.33999E+00   0.29929E-03   0.18419E-28   0.51082E-33
TOTAL      0.11360E+04                 0.36058E+05
```

## APPENDIX 4.8 -- TEST PROBLEM 4 -- AMOCO CORRELATION

```
     ***** PROBLEM STATEMENT *****


TYPE OF COLUMN       3

NO. OF PLATES      14

PRESSURE OF CONDENSER (PSIA)              25.00

PRESSURE AT TOP PLATE (PSIA)              27.00

PRESSURE DROP PER PLATE (PSIA)             0.3333

NO. OF FEEDS       1

   ENTERING PLATE OF FEED 1       2
   FEED QUANTITY        0.64652E+04
   PRESSURE OF FEED            48.00
   TEMPERATURE OF FEED (F)          180.00

NO. OF INTER COOLERS OR HEATERS        1

   PLATE NO. OF INTER COOLER OR HEATER 1      14
   HEAT LOAD OF INTER COOLER OR HEATER      0.16171E+08
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.11572E+01
TEMPERATURE
 0.55960E+03 0.67960E+03 0.69160E+03 0.69360E+03 0.69560E+03
 0.69760E+03 0.69960E+03 0.70160E+03 0.70360E+03 0.70560E+03
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03
VAPOUR FLOW RATE
 0.16000E+03 0.40000E+03 0.70000E+03 0.85000E+03 0.90000E+03
 0.90500E+03 0.91000E+03 0.91500E+03 0.92000E+03 0.92500E+03
 0.93000E+03 0.93500E+03 0.94000E+03 0.94500E+03

 1   SUM OF SQUARES OF RESIDUALS  0.46926E+00
TEMPERATURE
 0.55960E+03 0.67905E+03 0.70076E+03 0.71303E+03 0.71873E+03
 0.71886E+03 0.71594E+03 0.71272E+03 0.71057E+03 0.70978E+03
 0.71006E+03 0.71101E+03 0.71235E+03 0.71389E+03
VAPOUR FLOW RATE
 0.16293E+03 0.39896E+03 0.10727E+04 0.16067E+04 0.18000E+04
 0.17063E+04 0.15050E+04 0.13008E+04 0.11473E+04 0.10489E+04
 0.99322E+03 0.96599E+03 0.95767E+03 0.96398E+03

 2   SUM OF SQUARES OF RESIDUALS  0.43449E-01
TEMPERATURE
 0.55960E+03 0.67970E+03 0.69903E+03 0.70884E+03 0.71371E+03
 0.71378E+03 0.71207E+03 0.71081E+03 0.71054E+03 0.71100E+03
 0.71176E+03 0.71260E+03 0.71346E+03 0.71438E+03
VAPOUR FLOW RATE
 0.15497E+03 0.38493E+03 0.86282E+03 0.81415E+03 0.90000E+03
 0.97660E+03 0.10015E+04 0.10030E+04 0.10024E+04 0.99370E+03
 0.97804E+03 0.96679E+03 0.96767E+03 0.98765E+03

 3   SUM OF SQUARES OF RESIDUALS  0.36742E-02
TEMPERATURE
 0.55960E+03 0.67421E+03 0.69542E+03 0.70229E+03 0.70587E+03
 0.70757E+03 0.70826E+03 0.70889E+03 0.70970E+03 0.71057E+03
 0.71143E+03 0.71225E+03 0.71305E+03 0.71422E+03
VAPOUR FLOW RATE
 0.15331E+03 0.31629E+03 0.65657E+03 0.81270E+03 0.84425E+03
 0.88024E+03 0.90572E+03 0.92346E+03 0.92999E+03 0.93134E+03
 0.93359E+03 0.93771E+03 0.94532E+03 0.95267E+03
 4   SUM OF SQUARES OF RESIDUALS  0.11725E-02
TEMPERATURE
 0.55960E+03 0.67840E+03 0.69825E+03 0.70407E+03 0.70615E+03
 0.70745E+03 0.70848E+03 0.70935E+03 0.71015E+03 0.71092E+03
 0.71167E+03 0.71241E+03 0.71316E+03 0.71430E+03
VAPOUR FLOW RATE
 0.15575E+03 0.36490E+03 0.80808E+03 0.95032E+03 0.96431E+03
 0.96117E+03 0.95860E+03 0.95150E+03 0.94699E+03 0.94598E+03
 0.94716E+03 0.94958E+03 0.95119E+03 0.95078E+03

 5   SUM OF SQUARES OF RESIDUALS  0.71906E-04
TEMPERATURE
 0.55960E+03 0.67569E+03 0.69612E+03 0.70293E+03 0.70550E+03
 0.70700E+03 0.70813E+03 0.70907E+03 0.70993E+03 0.71074E+03
 0.71153E+03 0.71231E+03 0.71309E+03 0.71426E+03
VAPOUR FLOW RATE
 0.15444E+03 0.33694E+03 0.69902E+03 0.86897E+03 0.91187E+03
 0.92344E+03 0.92873E+03 0.93028E+03 0.93220E+03 0.93525E+03
 0.93901E+03 0.94309E+03 0.94656E+03 0.94865E+03

 6   SUM OF SQUARES OF RESIDUALS  0.16010E-04
TEMPERATURE
 0.55960E+03 0.67545E+03 0.69547E+03 0.70248E+03 0.70531E+03
 0.70691E+03 0.70807E+03 0.70904E+03 0.70992E+03 0.71075E+03
 0.71154E+03 0.71233E+03 0.71311E+03 0.71426E+03
VAPOUR FLOW RATE
 0.15483E+03 0.34149E+03 0.70823E+03 0.86014E+03 0.90241E+03
 0.91520E+03 0.92123E+03 0.92634E+03 0.93100E+03 0.93532E+03
 0.93936E+03 0.94311E+03 0.94649E+03 0.94903E+03

 7   SUM OF SQUARES OF RESIDUALS  0.10801E-04
TEMPERATURE
 0.55960E+03 0.67563E+03 0.69577E+03 0.70267E+03 0.70543E+03
 0.70699E+03 0.70813E+03 0.70909E+03 0.70995E+03 0.71077E+03
 0.71156E+03 0.71233E+03 0.71311E+03 0.71427E+03
VAPOUR FLOW RATE
 0.15476E+03 0.34281E+03 0.72096E+03 0.87085E+03 0.90667E+03
 0.91626E+03 0.92123E+03 0.92532E+03 0.92939E+03 0.93355E+03
 0.93772E+03 0.94176E+03 0.94549E+03 0.94839E+03
```

```
     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS   7

REFLUX RATIO          1.21519

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.480E+02 PSIA    0.180E+03 F    0.373E+08 BTU     1.0

*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP    LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO.     PSIA     F      LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1      25.00  100.00  0.18806E+03   0.15476E+03 -0.23475E+07
  2      27.00  216.03  0.70314E+04   0.34281E+03  0.0
  3      27.33  236.17  0.71813E+04   0.72096E+03  0.0
  4      27.67  243.07  0.72171E+04   0.87085E+03  0.0
  5      28.00  245.83  0.72267E+04   0.90667E+03  0.0
  6      28.33  247.39  0.72317E+04   0.91626E+03  0.0
  7      28.67  248.53  0.72358E+04   0.92123E+03  0.0
  8      29.00  249.49  0.72399E+04   0.92532E+03  0.0
  9      29.33  250.35  0.72440E+04   0.92939E+03  0.0
 10      29.67  251.17  0.72482E+04   0.93355E+03  0.0
 11      30.00  251.96  0.72522E+04   0.93772E+03  0.0
 12      30.33  252.73  0.72559E+04   0.94176E+03  0.0
 13      30.67  253.51  0.72588E+04   0.94549E+03  0.0
 14      31.00  254.67  0.63104E+04   0.94839E+03  0.16171E+08
```

```
*** MATERIAL BALANCES ***

FEEDS

                 PLATE NO.    2                  PLATE NO.
             LB MOL/TIME    MOL FRAC     LB MOL/TIME    MOL FRAC
H2S          0.37820E+02   0.58498E-02
CO2          0.12371E+03   0.19135E-01
DEA          0.29088E+03   0.44991E-01
H2O          0.60124E+04   0.92995E+00
METHANE      0.43000E+00   0.66510E-04
ETHANE       0.30000E-01   0.46402E-05
PROPANE      0.10000E-01   0.15467E-05
TOTAL        0.64652E+04

PRODUCTS

                 TOP PRODUCT                    BOTTOM PRODUCT
             LB MOL/TIME    MOL FRAC     LB MOL/TIME    MOL FRAC
H2S          0.37343E+02   0.24130E+00   0.47220E+00   0.74829E-04
CO2          0.11109E+03   0.71784E+00   0.12605E+02   0.19975E-02
DEA          0.51058E-08   0.32993E-10   0.29088E+03   0.46095E-01
H2O          0.58535E+01   0.37824E-01   0.60065E+04   0.95183E+00
METHANE      0.42994E+00   0.27782E-02   0.39749E-27   0.62990E-31
ETHANE       0.29996E-01   0.19383E-03   0.25954E-28   0.41129E-32
PROPANE      0.99987E-02   0.64609E-04   0.81276E-29   0.12880E-32
TOTAL        0.15476E+03                 0.63104E+04
```

APPENDIX 4.9 -- TEST PROBLEM 5 -- NASIR CORRELATION

```
     ***** PROBLEM STATEMENT *****


     TYPE OF COLUMN       1

     NO. OF PLATES       8

     PRESSURE AT TOP PLATE (PSIA)          150.00

     PRESSURE DROP PER PLATE (PSIA)          0.0

     NO. OF FEEDS       3

        ENTERING PLATE OF FEED 1       1
        FEED QUANTITY       0.69583E+03
        PRESSURE OF FEED          150.00
        TEMPERATURE OF FEED (F)          100.00

        ENTERING PLATE OF FEED 2       3
        FEED QUANTITY       0.28612E+04
        PRESSURE OF FEED          150.00
        TEMPERATURE OF FEED (F)          120.00

        ENTERING PLATE OF FEED 3       8
        FEED QUANTITY       0.19686E+04
        PRESSURE OF FEED          150.00
        TEMPERATURE OF FEED (F)           95.00

   PHYSICAL PARAMETERS
     KGA=  0.100E-05  KLO=  0.330E-01  AS(CM2/CM3)  0.430E+01
     XSECT AREA(CM2)  0.690E+04  WEIR HEIGHT(CM)  0.130E+02
```

6

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS . 0.38013E+01
TEMPERATURE
 0.56960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03
 0.57960E+03 0.57960E+03 0.57960E+03
VAPOUR FLOW RATE
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04
 0.19600E+04 0.19600E+04 0.19600E+04
H2S EFFICIENCY
 0.94167E+00 0.90612E+00 0.25987E+01 0.25987E+01 0.25987E+01
 0.25987E+01 0.21026E+02 0.20494E+02
CO2 EFFICIENCY
 0.41079E+01 0.23695E+01 0.42008E+02 0.42008E+02 0.42008E+02
 0.42008E+02 0.56385E+02 0.47435E+04

 1   SUM OF SQUARES OF RESIDUALS  0.35561E-01
TEMPERATURE
 0.59328E+03 0.61111E+03 0.56416E+03 0.56408E+03 0.56381E+03
 0.56291E+03 0.55992E+03 0.54587E+03
VAPOUR FLOW RATE
 0.19669E+04 0.19795E+04 0.19526E+04 0.19524E+04 0.19523E+04
 0.19518E+04 0.19495E+04 0.19706E+04
H2S EFFICIENCY
 0.85137E+00 0.81081E+00 0.81510E+00 0.81513E+00 0.81515E+00
 0.81523E+00 0.10892E+01 0.44576E+01
CO2 EFFICIENCY
 0.48516E+00 0.36059E+00 0.26116E+00 0.26091E+00 0.26004E+00
 0.25713E+00 0.63609E+02 0.17565E+04

 2   SUM OF SQUARES OF RESIDUALS  0.76671E-02
TEMPERATURE
 0.56327E+03 0.55701E+03 0.57553E+03 0.57545E+03 0.57540E+03
 0.57593E+03 0.58099E+03 0.57777E+03
VAPOUR FLOW RATE
 0.19469E+04 0.19244E+04 0.19592E+04 0.19590E+04 0.19590E+04
 0.19591E+04 0.19611E+04 0.19624E+04
H2S EFFICIENCY
 0.99165E+00 0.26609E+01 0.90759E+00 0.90695E+00 0.90163E+00
 0.11319E+01 0.12313E+01 0.19680E+01
CO2 EFFICIENCY
 0.90456E+00 0.81149E+00 0.38273E+00 0.38122E+00 0.37441E+00
 0.43676E+02 0.22173E+03 0.21577E+03
 3   SUM OF SQUARES OF RESIDUALS  0.17042E-02
TEMPERATURE
 0.57182E+03 0.59192E+03 0.58210E+03 0.58217E+03 0.58243E+03
 0.58311E+03 0.58320E+03 0.57829E+03
VAPOUR FLOW RATE
 0.19569E+04 0.19629E+04 0.19638E+04 0.19637E+04 0.19638E+04
 0.19648E+04 0.19672E+04 0.19684E+04
H2S EFFICIENCY
 0.11050E+01 0.16033E+01 0.94064E+00 0.93923E+00 0.97432E+00
 0.10425E+01 0.13188E+01 0.19516E+01
CO2 EFFICIENCY
 0.37752E+00 0.53995E+00 0.48877E+00 0.48475E+00 0.19473E+02
 0.15075E+03 0.16890E+03 0.21065E+03

 4   SUM OF SQUARES OF RESIDUALS  0.89964E-04
TEMPERATURE
 0.57298E+03 0.57706E+03 0.57926E+03 0.57947E+03 0.58005E+03
 0.58090E+03 0.58029E+03 0.57538E+03
VAPOUR FLOW RATE
 0.19579E+04 0.19588E+04 0.19627E+04 0.19627E+04 0.19633E+04
 0.19649E+04 0.19657E+04 0.19668E+04
H2S EFFICIENCY
 0.15317E+01 0.21714E+01 0.99759E+00 0.10075E+01 0.10297E+01
 0.11132E+01 0.13750E+01 0.20676E+01
CO2 EFFICIENCY
 0.71607E+00 0.10933E+01 0.67922E+00 0.15311E+02 0.12567E+03
 0.14979E+03 0.20011E+03 0.25155E+03

 5   SUM OF SQUARES OF RESIDUALS  0.20732E-04
TEMPERATURE
 0.57134E+03 0.57856E+03 0.57967E+03 0.58007E+03 0.58077E+03
 0.58101E+03 0.58044E+03 0.57576E+03
VAPOUR FLOW RATE
 0.19572E+04 0.19613E+04 0.19630E+04 0.19631E+04 0.19642E+04
 0.19648E+04 0.19657E+04 0.19668E+04
H2S EFFICIENCY
 0.17583E+01 0.21306E+01 0.99555E+00 0.10040E+01 0.10272E+01
 0.10992E+01 0.13565E+01 0.20535E+01
CO2 EFFICIENCY
 0.87513E+00 0.12371E+01 0.10332E+02 0.87733E+02 0.10923E+03
 0.15374E+03 0.20500E+03 0.24767E+03
 6   SUM OF SQUARES OF RESIDUALS  0.18246E-05
TEMPERATURE
 0.57249E+03 0.57775E+03 0.57961E+03 0.58011E+03 0.58043E+03
 0.58070E+03 0.58016E+03 0.57556E+03
VAPOUR FLOW RATE
 0.19577E+04 0.19609E+04 0.19630E+04 0.19635E+04 0.19640E+04
 0.19646E+04 0.19655E+04 0.19668E+04
H2S EFFICIENCY
 0.16945E+01 0.21532E+01 0.99901E+00 0.10065E+01 0.10255E+01
 0.10961E+01 0.13627E+01 0.20614E+01
CO2 EFFICIENCY
 0.87018E+00 0.14533E+02 0.60327E+02 0.77045E+02 0.11192E+03
 0.15726E+03 0.20648E+03 0.25011E+03
```

```
     ***** COMPUTED RESULTS *****

   NUMBER OF ITERATIONS    6

   PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

    0.150E+03 PSIA    0.100E+03 F    0.290E+07 BTU     1.0

    0.150E+03 PSIA    0.120E+03 F    0.119E+08 BTU     1.0

    0.150E+03 PSIA    0.950E+02 F    0.128E+08 BTU     0.0

   *** STAGE VARIABLES ***

   PLATE   PRESSURE  TEMP    LIQUID FLOW    VAPOUR FLOW    HEAT DUTY
    NO.      PSIA     F      LB MOL/TIME    LB MOL/TIME    BTU/TIME
     1     150.00  112.89   0.69897E+03    0.19577E+04    0.0
     2     150.00  118.16   0.70110E+03    0.19609E+04    0.0
     3     150.00  120.02   0.35628E+04    0.19630E+04    0.0
     4     150.00  120.51   0.35633E+04    0.19635E+04    0.0
     5     150.00  120.83   0.35639E+04    0.19640E+04    0.0
     6     150.00  121.10   0.35648E+04    0.19646E+04    0.0
     7     150.00  120.56   0.35661E+04    0.19655E+04    0.0
     8     150.00  115.96   0.35679E+04    0.19668E+04    0.0
```

```
*** MATERIAL BALANCES ***

FEEDS

                 PLATE NO.    1                   PLATE NO.    3
            LB MOL/TIME     MOL FRAC       LB MOL/TIME     MOL FRAC
H2S         0.12800E+01   0.18395E-02     0.54300E+02   0.18978E-01
CO2         0.15700E+01   0.22563E-02     0.63000E+01   0.22019E-02
MEA         0.62050E+02   0.89174E-01     0.25000E+03   0.87377E-01
WATER       0.63093E+03   0.90673E+00     0.25500E+04   0.89124E+00
HYDROGEN    0.0           0.0             0.0           0.0
NITROGEN    0.0           0.0             0.0           0.0
METHANE     0.0           0.0             0.0           0.0
ETHANE      0.0           0.0             0.16000E+00   0.55921E-04
PROPANE     0.0           0.0             0.42000E+00   0.14679E-03
N-BUTANE    0.0           0.0             0.0           0.0
I-BUTANE    0.0           0.0             0.0           0.0
TOTAL       0.69583E+03                   0.28612E+04

                 PLATE NO.    8                   PLATE NO.
            LB MOL/TIME     MOL FRAC       LB MOL/TIME     MOL FRAC
H2S         0.18700E+02   0.94989E-02
CO2         0.29500E+01   0.14985E-02
MEA         0.0           0.0
WATER       0.59100E+01   0.30021E-02
HYDROGEN    0.62997E+03   0.32000E+00
NITROGEN    0.29530E+02   0.15000E-01
METHANE     0.78155E+03   0.39700E+00
ETHANE      0.35436E+03   0.18000E+00
PROPANE     0.12402E+03   0.62997E-01
N-BUTANE    0.19700E+01   0.10007E-02
I-BUTANE    0.19690E+02   0.10002E-01
TOTAL       0.19686E+04

PRODUCTS

                  TOP PRODUCT                  BOTTOM PRODUCT
            LB MOL/TIME     MOL FRAC       LB MOL/TIME     MOL FRAC
H2S         0.63932E-01   0.32656E-04     0.74221E+02   0.20802E-01
CO2         0.22796E-03   0.11644E-06     0.10823E+02   0.30335E-02
MEA         0.39981E-01   0.20422E-04     0.31201E+03   0.87448E-01
WATER       0.16523E+02   0.84399E-02     0.31703E+04   0.88856E+00
HYDROGEN    0.62983E+03   0.32172E+00     0.16325E+00   0.45756E-04
NITROGEN    0.29525E+02   0.15081E-01     0.54106E-02   0.15165E-05
METHANE     0.78127E+03   0.39907E+00     0.26842E+00   0.75231E-04
ETHANE      0.35443E+03   0.18104E+00     0.91658E-01   0.25689E-04
PROPANE     0.12438E+03   0.63533E-01     0.35386E-01   0.99176E-05
N-BUTANE    0.19699E+01   0.10062E-02     0.32513E-04   0.91125E-08
I-BUTANE    0.19689E+02   0.10057E-01     0.32496E-03   0.91079E-07
TOTAL       0.19577E+04                   0.35679E+04
```

# APPENDIX 5

# EQUILIBRIUM AND ENTHALPY DATA FOR EXTRACTIVE DISTILLATION PROBLEM

# APPENDIX 5

## Equilibrium and Enthalpy Data for Extractive Distillation Problem

### (a) Equilibrium K-ratios

At low pressures, far from critical conditions, the K-value of component i may be expressed by:

$$K_i = \gamma_i \frac{p_i^*}{P_T} \tag{A5-1}$$

where:

$\gamma_i$ is the activity coefficient

$p_i^*$ is the intrinsic vapour pressure of the pure component

$P_T$ is the total pressure.

For a three component system, a third order Margules' expression may be used, namely equation (A5-2). By cyclically altering subscripts, similar expressions are obtained for $\ell n\ \gamma_2$ and $\ell n\ \gamma_3$.

$$\begin{aligned} \ell n\ \gamma_1 = {} & x_2^{\,2}\{a_{12} + 2x_1\,(a_{21} - a_{12})\} + x_3^{\,2}\,\{a_{13} + 2x_1(a_{31} - a_{13})\} \\ & + x_2\,x_3\,\{0.5(a_{12} + a_{21} + a_{13} + a_{31} - a_{23} - a_{32}) \\ & + x_1(a_{21} - a_{12} + a_{31} - a_{13}) + (x_2 - x_3)(a_{23} - a_{32}) - (1 - 2x_1)c_{123}\} \end{aligned} \tag{A5-2}$$

The third order constants are as follows[13], with subscripts 1,2,3 denoting acetone, acetonitrile and water respectively.

$a_{12} = 0.0482 \quad a_{23} = 0.8145 \quad a_{31} = 0.6867$

$a_{21} = -0.0447 \quad a_{32} = 0.7375 \quad a_{13} = 0.8484$

$c_{123} = 0.3462$

The intrinsic vapour pressure of component *i* is given by Antoine's equation[13]:

$$\log p_i^* = A_i - \frac{B_i}{(T_c + C_i)} \qquad \text{(A5-3)}$$

where $T_c$ is the temperature (°C)

$A_i, B_i, C_i$ are Antoine's constants. For the system acetone-acetonitrile-water they are[13]:

| Component, i | $A_i$ | $B_i$ | $C_i$ |
|---|---|---|---|
| acetone | 7.23967 | 1279.870 | 237.5 |
| acetonitrile | 7.24299 | 1397.929 | 238.894 |
| water | 7.96681 | 1668.210 | 228.0 |

The partial derivatives of $K_i$ with respect to T and $x_i$ are given by equations (A5-4) and (A5-5):

$$\frac{\partial K_i}{\partial T} = \frac{\gamma_i}{P_T}\frac{\partial p_i^*}{\partial T} + \frac{p_i}{P_T}\frac{\partial \gamma_i}{\partial T} \qquad \text{(A5-4)}$$

$$\frac{\partial K_i}{\partial x_i} = \frac{p_i^*}{P_T} \frac{\partial \gamma_i}{\partial x_i} \qquad \text{(A5-5)}$$

However, for the purposes of linearization, $\frac{\partial \gamma_i}{\partial T}$ is considered negligible and $\frac{\partial K_i}{\partial T}$ approximated as:

$$\frac{\partial K_i}{\partial T} = \frac{\gamma_i}{P_T} \frac{\partial p_i^*}{\partial T} \qquad \text{(A5-6)}$$

From equation (A5-2), $\frac{\partial \gamma_1}{\partial x_1}$ is given by the following:

$$\frac{\partial \gamma_1}{\partial x_1} = \gamma_1 \{ 2x_2^2(a_{21} - a_{12}) + 2x_3^2(a_{31} - a_{13}) + x_2 x_3[(a_{21}-a_{12}+a_{31}-a_{13}) + 2c_{123}] \qquad \text{(A5-7)}$$

Similar expressions apply for $\frac{\partial \gamma_2}{\partial x_2}$ and $\frac{\partial \gamma_3}{\partial x_3}$.

(b) Enthalpy Data

Liquid and vapour enthalpy are given by the following:

$$h = \sum_{i=1}^{NCP} hc_i \; x_i \; XM_i \; (T-T_{ref}) \qquad \text{(A5-8)}$$

$$H = \sum_{i=1}^{NCP} y_i \; XM_i \; [hc_i(T-T_{ref}) + h_{vap,i}] \qquad \text{(A5-9)}$$

where $hc_i$, $XM_i$, $h_{vap,i}$ are respectively the average heat capacity, molecular weight and average heat of vapourization of component $i$, T is the temperature (°C), and $T_{ref}$ is the reference temperature, conveniently chosen as 0°C. Values of $hc_i$, $XM_i$ and $h_{vap,i}$ are as follows:

| | Heat Capacity (cal/g°C) | Molecular Weight | Heat of Vapourization (cal/g) |
|---|---|---|---|
| acetone | 0.54 | 58.08 | 120.0 |
| acetonitrile | 0.54 | 41.05 | 120.0 |
| water | 1.00 | 18.02 | 550.0 |

Finally, the partial derivatives of the liquid and vapour enthalpies with respect to temperature are:

$$\frac{\partial h}{\partial T} = \sum_{i=1}^{NCP} hc_i \; x_i \; XM_i \; / \; 1.8 \qquad \text{(A5-10)}$$

$$\frac{\partial H}{\partial T} = \sum_{i=1}^{NCP} hc_i \; y_i \; XM_i \; / \; 1.8 \qquad \text{(A5-11)}$$

where T is in °R.

# APPENDIX 6

## COMPUTER PRINTOUTS FOR EXAMPLE PROBLEMS USING LINKED COLUMN ALGORITHM

V

```
  APPENDIX 6.1 -- THERMALLY COUPLED DISTILLATION SYSTEM

  ** PROBLEM STATEMENT **

      COLUMN NO 1 IS DISTILLATION COL.
NO OF PLATES= 30
COL PRESSURE     235.00 PSIA
PRESSURE DROP      0.0  PER PLATE
REBOILER VAPOUR    6850.00 MOLES
REFLUX RATIO          2.500

      COLUMN NO 2 IS ABSORPTION COL.
NO OF PLATES= 20
COL PRESSURE     235.00 PSIA
PRESSURE DROP      0.0  PER PLATE

 NO. OF FEEDS          1

   FEED 1 IS ON TO PLATE 15
     QUANTITY        0.40800E+04
     PRESSURE           235.00
     TEMP (F)           150.00
     ENTHALPY        0.63100E+07

 NO. OF LIQUID SIDE STREAMS          1

   STREAM 1 LEAVES PLATE  5
     QUANTITY        0.25000E+04

 NO. OF VAPOUR SIDE STREAMS          2

   STREAM 1 LEAVES PLATE 25
     QUANTITY        0.30000E+04

   STREAM 2 LEAVES PLATE 40
     QUANTITY        0.12096E+04

 NO. OF INTERCOOLERS OR HEATERS          1

   INTERCOOLER OR HEATER 1 IS ON PLATE 30
     HEAT LOAD IS A VARIABLE


 *** STREAM CONNECTIONS ***

   LEAVING     LEAVING     STREAM    ENTERING   ENTERING     ENTERING
   STREAM NO   STAGE NO    FLUID     FRACTION   STREAM NO    STAGE NO

       1           5         1         1.00         3            31
       2          25         2         1.00         4            50
       3          31         4         1.00         1             5
       4          50         3         1.00         2            25

   STREAM FLUID    1=LIQUID SIDE STREAM  2=VAPOUR SIDE STREAM
                   3=LIQUID PRODUCT  4=VAPOUR PRODUCT
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.23241E+01
    (MAT. BAL.  0.23161E+01   HEAT BAL.  0.79483E-02)
TEMPERATURE (R)                  0.58560E+03 0.58960E+03 0.59360E+03
 0.58160E+03 0.58360E+03 0.58560E+03 0.60560E+03 0.60760E+03
 0.59760E+03 0.60160E+03 0.60360E+03 0.61560E+03 0.62360E+03
 0.60960E+03 0.61160E+03 0.61360E+03 0.65560E+03 0.66360E+03
 0.63160E+03 0.63960E+03 0.64760E+03 0.69960E+03 0.71160E+03
 0.67160E+03 0.67960E+03 0.68760E+03 0.75960E+03 0.78460E+03
 0.72360E+03 0.73560E+03 0.74760E+03 0.62060E+03 0.63260E+03
 0.59660E+03 0.60460E+03 0.61260E+03 0.67260E+03 0.68060E+03
 0.64460E+03 0.65660E+03 0.66460E+03 0.70360E+03 0.70560E+03
 0.68860E+03 0.69660E+03 0.70160E+03 0.71360E+03 0.71560E+03
 0.70760E+03 0.70960E+03 0.71160E+03
VAPOUR FLOW RATE                 0.76500E+04 0.76000E+04 0.75500E+04
 0.22072E+04 0.77252E+04 0.76500E+04 0.50000E+04 0.50000E+04
 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04
 0.50000E+04 0.50000E+04 0.50000E+04 0.48000E+04 0.48000E+04
 0.48000E+04 0.48000E+04 0.48000E+04 0.48000E+04 0.48000E+04
 0.48000E+04 0.48000E+04 0.48000E+04 0.75000E+04 0.68500E+04
 0.75000E+04 0.75000E+04 0.75000E+04 0.22000E+04 0.22000E+04
 0.22000E+04 0.22000E+04 0.22000E+04 0.22000E+04 0.22000E+04
 0.22000E+04 0.22000E+04 0.22000E+04 0.31000E+04 0.31000E+04
 0.31000E+04 0.31000E+04 0.31000E+04 0.31000E+04 0.31000E+04
 0.31000E+04 0.31000E+04 0.31000E+04

 1   SUM OF SQUARES OF RESIDUALS  0.62283E-02
    (MAT. BAL.  0.56247E-02   HEAT BAL.  0.60354E-03)
TEMPERATURE (R)                  0.58494E+03 0.58766E+03 0.59101E+03
 0.58038E+03 0.58283E+03 0.58494E+03 0.60509E+03 0.60745E+03
 0.59504E+03 0.59898E+03 0.60228E+03 0.61703E+03 0.62436E+03
 0.60949E+03 0.61144E+03 0.61370E+03 0.65352E+03 0.66256E+03
 0.62945E+03 0.63646E+03 0.64461E+03 0.69962E+03 0.71320E+03
 0.67123E+03 0.67963E+03 0.68862E+03 0.76300E+03 0.78661E+03
 0.72438E+03 0.73648E+03 0.74841E+03 0.60718E+03 0.61585E+03
 0.59215E+03 0.59578E+03 0.60061E+03 0.66154E+03 0.67367E+03
 0.62575E+03 0.63698E+03 0.64901E+03 0.69302E+03 0.69628E+03
 0.67946E+03 0.68527E+03 0.68948E+03 0.70702E+03 0.70970E+03
 0.69929E+03 0.70205E+03 0.70459E+03
VAPOUR FLOW RATE                 0.74474E+04 0.74143E+04 0.73749E+04
 0.21304E+04 0.74562E+04 0.74474E+04 0.49791E+04 0.49451E+04
 0.50942E+04 0.50502E+04 0.50148E+04 0.47495E+04 0.45881E+04
 0.49110E+04 0.48736E+04 0.48250E+04 0.48727E+04 0.48943E+04
 0.48476E+04 0.48367E+04 0.48526E+04 0.48615E+04 0.48454E+04
 0.49116E+04 0.49143E+04 0.48978E+04 0.74069E+04 0.68500E+04
 0.78188E+04 0.77288E+04 0.76495E+04 0.22170E+04 0.22011E+04
 0.22550E+04 0.22341E+04 0.22279E+04 0.20264E+04 0.19870E+04
 0.21831E+04 0.21458E+04 0.20887E+04 0.31451E+04 0.31330E+04
 0.32030E+04 0.31609E+04 0.31549E+04 0.30742E+04 0.30450E+04
 0.31210E+04 0.31082E+04 0.30934E+04
 2   SUM OF SQUARES OF RESIDUALS  0.24[illegible]-02
    (MAT. BAL.   0.87044E-03   HEAT BA[illegible] 0.15720E-02)
TEMPERATURE (R)
 0.58068E+03 0.58232E+03 0.58409E+03 0.58635E+03 0.58932E+03
 0.59344E+03 0.59733E+03 0.60070E+03 0.60347E+03 0.60573E+03
 0.60766E+03 0.60950E+03 0.61167E+03 0.61490E+03 0.62205E+03
 0.62689E+03 0.63316E+03 0.64103E+03 0.65006E+03 0.65954E+03
 0.66893E+03 0.67840E+03 0.68905E+03 0.70255E+03 0.71962E+03
 0.73267E+03 0.74453E+03 0.75564E+03 0.76903E+03 0.79298E+03
 0.59230E+03 0.59686E+03 0.60419E+03 0.61506E+03 0.62913E+03
 0.64460E+03 0.65857E+03 0.66902E+03 0.67648E+03 0.68417E+03
 0.69144E+03 0.69819E+03 0.70420E+03 0.70914E+03 0.71281E+03
 0.71525E+03 0.71663E+03 0.71727E+03 0.71753E+03 0.71793E+03
VAPOUR FLOW RATE
 0.22176E+04 0.77614E+04 0.77150E+04 0.76512E+04 0.75697E+04
 0.50758E+04 0.50144E+04 0.49648E+04 0.49266E+04 0.48975E+04
 0.48741E+04 0.48513E+04 0.48218E+04 0.47722E+04 0.46586E+04
 0.48349E+04 0.47887E+04 0.47400E+04 0.47073E+04 0.47037E+04
 0.47290E+04 0.47631E+04 0.47722E+04 0.47408E+04 0.46821E+04
 0.76089E+04 0.75720E+04 0.75307E+04 0.73592E+04 0.68500E+04
 0.24021E+04 0.23788E+04 0.23429E+04 0.22980E+04 0.22580E+04
 0.22330E+04 0.22259E+04 0.22153E+04 0.21883E+04 0.21334E+04
 0.32674E+04 0.32132E+04 0.31732E+04 0.31431E+04 0.31218E+04
 0.31063E+04 0.30942E+04 0.30832E+04 0.30713E+04 0.30534E+04

 3   SUM OF SQUARES OF RESIDUALS  0.12708E-02
    (MAT. BAL.   0.26290E-03   HEAT BAL.  0.10074E-02)
TEMPERATURE (R)
 0.58150E+03 0.58380E+03 0.58638E+03 0.58969E+03 0.59383E+03
 0.59943E+03 0.60419E+03 0.60784E+03 0.61050E+03 0.61244E+03
 0.61396E+03 0.61541E+03 0.61720E+03 0.62002E+03 0.62641E+03
 0.63440E+03 0.64430E+03 0.65542E+03 0.66631E+03 0.67566E+03
 0.68324E+03 0.69008E+03 0.69798E+03 0.70868E+03 0.72257E+03
 0.73393E+03 0.74470E+03 0.75541E+03 0.76898E+03 0.79332E+03
 0.59718E+03 0.60225E+03 0.60974E+03 0.61974E+03 0.63145E+03
 0.64348E+03 0.65473E+03 0.66466E+03 0.67386E+03 0.68415E+03
 0.69256E+03 0.69947E+03 0.70492E+03 0.70905E+03 0.71206E+03
 0.71423E+03 0.71583E+03 0.71708E+03 0.71823E+03 0.71968E+03
VAPOUR FLOW RATE
 0.22237E+04 0.77828E+04 0.77422E+04 0.76823E+04 0.76060E+04
 0.52512E+04 0.51907E+04 0.51457E+04 0.51121E+04 0.50858E+04
 0.50621E+04 0.50370E+04 0.50040E+04 0.49513E+04 0.48309E+04
 0.50466E+04 0.50475E+04 0.50643E+04 0.51060E+04 0.51620E+04
 0.52041E+04 0.52019E+04 0.51394E+04 0.50178E+04 0.48747E+04
 0.77406E+04 0.76681E+04 0.75960E+04 0.74032E+04 0.68500E+04
 0.22649E+04 0.22381E+04 0.21957E+04 0.21386E+04 0.20709E+04
 0.20040E+04 0.19571E+04 0.19499E+04 0.19792E+04 0.19756E+04
 0.31490E+04 0.31057E+04 0.30656E+04 0.30351E+04 0.30163E+04
 0.30080E+04 0.30081E+04 0.30127E+04 0.30178E+04 0.30176E+04
 4   SUM OF SQUARES OF RESIDUALS  0.75071E-03
    (MAT. BAL.  0.13282E-03   HEAT BAL.  0.61788E-03)
TEMPERATURE (R)
 0.58140E+03 0.58361E+03 0.58605E+03 0.58910E+03 0.59288E+03
 0.59700E+03 0.60066E+03 0.60366E+03 0.60605E+03 0.60795E+03
 0.60959E+03 0.61120E+03 0.61319E+03 0.61628E+03 0.62320E+03
 0.62889E+03 0.63634E+03 0.64553E+03 0.65565E+03 0.66545E+03
 0.67423E+03 0.68239E+03 0.69135E+03 0.70290E+03 0.71788E+03
 0.73011E+03 0.74176E+03 0.75326E+03 0.76743E+03 0.79214E+03
 0.59809E+03 0.60594E+03 0.61690E+03 0.63004E+03 0.64311E+03
 0.65393E+03 0.66200E+03 0.66847E+03 0.67512E+03 0.68364E+03
 0.69097E+03 0.69707E+03 0.70190E+03 0.70554E+03 0.70819E+03
 0.71011E+03 0.71153E+03 0.71266E+03 0.71373E+03 0.71510E+03
VAPOUR FLOW RATE
 0.22180E+04 0.77632E+04 0.77089E+04 0.76334E+04 0.75397E+04
 0.50778E+04 0.50109E+04 0.49622E+04 0.49282E+04 0.49042E+04
 0.48847E+04 0.48644E+04 0.48364E+04 0.47884E+04 0.46732E+04
 0.48199E+04 0.47311E+04 0.46409E+04 0.45900E+04 0.46053E+04
 0.46747E+04 0.47519E+04 0.47902E+04 0.47743E+04 0.47284E+04
 0.76657E+04 0.76330E+04 0.75821E+04 0.73969E+04 0.68500E+04
 0.23554E+04 0.23212E+04 0.22780E+04 0.22378E+04 0.22132E+04
 0.22045E+04 0.21978E+04 0.21802E+04 0.21439E+04 0.20894E+04
 0.32287E+04 0.31772E+04 0.31429E+04 0.31207E+04 0.31061E+04
 0.30946E+04 0.30841E+04 0.30737E+04 0.30605E+04 0.30413E+04

 5   SUM OF SQUARES OF RESIDUALS  0.11433E-03
    (MAT. BAL.  0.91650E-04   HEAT BAL.  0.22675E-04)
TEMPERATURE (R)
 0.58120E+03 0.58331E+03 0.58562E+03 0.58856E+03 0.59225E+03
 0.59721E+03 0.60151E+03 0.60494E+03 0.60756E+03 0.60958E+03
 0.61126E+03 0.61289E+03 0.61486E+03 0.61789E+03 0.62460E+03
 0.63122E+03 0.63952E+03 0.64914E+03 0.65904E+03 0.66821E+03
 0.67634E+03 0.68409E+03 0.69289E+03 0.70435E+03 0.71905E+03
 0.73099E+03 0.74230E+03 0.75345E+03 0.76722E+03 0.79142E+03
 0.59554E+03 0.60083E+03 0.60921E+03 0.62089E+03 0.63428E+03
 0.64677E+03 0.65688E+03 0.66508E+03 0.67290E+03 0.68217E+03
 0.68986E+03 0.69628E+03 0.70145E+03 0.70544E+03 0.70841E+03
 0.71059E+03 0.71223E+03 0.71352E+03 0.71471E+03 0.71618E+03
VAPOUR FLOW RATE
 0.22064E+04 0.77225E+04 0.76734E+04 0.76041E+04 0.75174E+04
 0.51144E+04 0.50529E+04 0.50079E+04 0.49755E+04 0.49511E+04
 0.49300E+04 0.49075E+04 0.48773E+04 0.48269E+04 0.47099E+04
 0.48899E+04 0.48438E+04 0.48011E+04 0.47856E+04 0.48081E+04
 0.48544E+04 0.48929E+04 0.48931E+04 0.48468E+04 0.47799E+04
 0.77013E+04 0.76554E+04 0.75923E+04 0.73996E+04 0.68500E+04
 0.23035E+04 0.22662E+04 0.22105E+04 0.21471E+04 0.20991E+04
 0.20823E+04 0.20882E+04 0.20937E+04 0.20809E+04 0.20460E+04
 0.31998E+04 0.31554E+04 0.31245E+04 0.31043E+04 0.30913E+04
 0.30819E+04 0.30737E+04 0.30655E+04 0.30550E+04 0.30383E+04
```

```
6   SUM OF SQUARES OF RESIDUALS  0.52946E-04
   (MAT. BAL.  0.17485E-06   HEAT BAL.  0.52771E-04)
TEMPERATURE (R)
 0.58141E+03 0.58366E+03 0.58617E+03 0.58933E+03 0.59325E+03
 0.59823E+03 0.60243E+03 0.60570E+03 0.60817E+03 0.61006E+03
 0.61166E+03 0.61322E+03 0.61515E+03 0.61815E+03 0.62481E+03
 0.63145E+03 0.63952E+03 0.64863E+03 0.65798E+03 0.66681E+03
 0.67499E+03 0.68306E+03 0.69224E+03 0.70404E+03 0.71893E+03
 0.73090E+03 0.74220E+03 0.75330E+03 0.76699E+03 0.79109E+03
 0.59699E+03 0.60265E+03 0.61086E+03 0.62144E+03 0.63325E+03
 0.64468E+03 0.65472E+03 0.66338E+03 0.67174E+03 0.68135E+03
 0.68914E+03 0.69562E+03 0.70087E+03 0.70494E+03 0.70801E+03
 0.71028E+03 0.71198E+03 0.71332E+03 0.71455E+03 0.71603E+03
VAPOUR FLOW RATE
 0.22014E+04 0.77051E+04 0.76573E+04 0.75908E+04 0.75079E+04
 0.51174E+04 0.50597E+04 0.50172E+04 0.49854E+04 0.49607E+04
 0.49384E+04 0.49148E+04 0.48833E+04 0.48316E+04 0.47136E+04
 0.49057E+04 0.48776E+04 0.48539E+04 0.48491E+04 0.48678E+04
 0.48976E+04 0.49179E+04 0.49055E+04 0.48504E+04 0.47788E+04
 0.76977E+04 0.76487E+04 0.75846E+04 0.73938E+04 0.68500E+04
 0.22963E+04 0.22627E+04 0.22140E+04 0.21572E+04 0.21074E+04
 0.20796E+04 0.20731E+04 0.20736E+04 0.20639E+04 0.20351E+04
 0.31949E+04 0.31522E+04 0.31207E+04 0.30992E+04 0.30847E+04
 0.30749E+04 0.30671E+04 0.30601E+04 0.30511E+04 0.30365E+04

7   SUM OF SQUARES OF RESIDUALS  0.55142E-05
   (MAT. BAL.  0.53997E-07   HEAT BAL.  0.54602E-05)
TEMPERATURE (R)
 0.58138E+03 0.58360E+03 0.58608E+03 0.58919E+03 0.59304E+03
 0.59787E+03 0.60198E+03 0.60521E+03 0.60766E+03 0.60957E+03
 0.61118E+03 0.61276E+03 0.61471E+03 0.61773E+03 0.62444E+03
 0.63082E+03 0.63866E+03 0.64762E+03 0.65696E+03 0.66592E+03
 0.67424E+03 0.68242E+03 0.69167E+03 0.70352E+03 0.71847E+03
 0.73052E+03 0.74190E+03 0.75307E+03 0.76681E+03 0.79096E+03
 0.59692E+03 0.60276E+03 0.61117E+03 0.62196E+03 0.63386E+03
 0.64523E+03 0.65510E+03 0.66362E+03 0.67183E+03 0.68129E+03
 0.68899E+03 0.69539E+03 0.70057E+03 0.70460E+03 0.70763E+03
 0.70988E+03 0.71155E+03 0.71288E+03 0.71410E+03 0.71558E+03
VAPOUR FLOW RATE
 0.22006E+04 0.77022E+04 0.76523E+04 0.75832E+04 0.74978E+04
 0.50957E+04 0.50374E+04 0.49952E+04 0.49644E+04 0.49403E+04
 0.49191E+04 0.48960E+04 0.48651E+04 0.48140E+04 0.46963E+04
 0.48841E+04 0.48544E+04 0.48354E+04 0.48389E+04 0.48645E+04
 0.48976E+04 0.49160E+04 0.48995E+04 0.48399E+04 0.47652E+04
 0.76825E+04 0.76350E+04 0.75744E+04 0.73889E+04 0.68500E+04
 0.23058E+04 0.22744E+04 0.22319E+04 0.21863E+04 0.21487E+04
 0.21259E+04 0.21145E+04 0.21048E+04 0.20867E+04 0.20520E+04
 0.32079E+04 0.31635E+04 0.31300E+04 0.31064E+04 0.30903E+04
 0.30787E+04 0.30699E+04 0.30616E+04 0.30521E+04 0.30369E+04
```

```
     ***** COMPUTED RESULTS *****

   NUMBER OF ITERATIONS   7

   PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

    1   235.00 PSIA   150.00 F    0.63100E+07 BTU    1.000

   *** STREAM CONNECTIONS ***

   LEAVING     LEAVING    STREAM   ENTERING   ENTERING    ENTERING
   STREAM NO   STAGE NO   FLUID    FRACTION   STREAM NO   STAGE NO

         1          5       1        1.00        3           31
         2         25       2        1.00        4           50
         3         31       4        1.00        1            5
         4         50       3        1.00        2           25

   STREAM FLUID    1=LIQUID SIDE STREAM   2=VAPOUR SIDE STREAM
                   3=LIQUID PRODUCT   4=VAPOUR PRODUCT
15:25:17 .03 RC=0
```

```
*** STAGE VARIABLES ***

PLATE  PRESSURE   TEMP     LIQUID FLOW    VAPOUR FLOW    HEAT DUTY
 NO      PSIA       F     LB MOL/TIME    LB MOL/TIME    BTU/TIME
  1     235.00   121.78   0.55016E+04    0.22006E+04   -0.33053E+08
  2     235.00   124.00   0.54517E+04    0.77022E+04    0.0
  3     235.00   126.48   0.53826E+04    0.76523E+04    0.0
  4     235.00   129.59   0.52972E+04    0.75832E+04    0.0
  5     235.00   133.44   0.27009E+04    0.74978E+04    0.0
  6     235.00   138.27   0.26426E+04    0.50957E+04    0.0
  7     235.00   142.38   0.26004E+04    0.50374E+04    0.0
  8     235.00   145.61   0.25695E+04    0.49952E+04    0.0
  9     235.00   148.06   0.25455E+04    0.49644E+04    0.0
 10     235.00   149.97   0.25243E+04    0.49403E+04    0.0
 11     235.00   151.58   0.25012E+04    0.49191E+04    0.0
 12     235.00   153.16   0.24702E+04    0.48960E+04    0.0
 13     235.00   155.11   0.24191E+04    0.48651E+04    0.0
 14     235.00   158.13   0.23015E+04    0.48140E+04    0.0
 15     235.00   164.84   0.65692E+04    0.46963E+04    0.0
 16     235.00   171.22   0.65396E+04    0.48841E+04    0.0
 17     235.00   179.06   0.65205E+04    0.48544E+04    0.0
 18     235.00   188.02   0.65240E+04    0.48354E+04    0.0
 19     235.00   197.36   0.65497E+04    0.48389E+04    0.0
 20     235.00   206.32   0.65828E+04    0.48645E+04    0.0
 21     235.00   214.64   0.66012E+04    0.48976E+04    0.0
 22     235.00   222.82   0.65846E+04    0.49160E+04    0.0
 23     235.00   232.07   0.65250E+04    0.48995E+04    0.0
 24     235.00   243.92   0.64503E+04    0.48399E+04    0.0
 25     235.00   258.87   0.83523E+04    0.47652E+04    0.0
 26     235.00   270.92   0.83047E+04    0.76825E+04    0.0
 27     235.00   282.30   0.82442E+04    0.76350E+04    0.0
 28     235.00   293.47   0.80587E+04    0.75744E+04    0.0
 29     235.00   307.21   0.75198E+04    0.73889E+04    0.0
 30     235.00   331.36   0.66977E+03    0.68500E+04    0.61639E+08
 --------------------------------------------------------------------
 31     235.00   137.32   0.24686E+04    0.23058E+04    0.0
 32     235.00   143.16   0.24261E+04    0.22744E+04    0.0
 33     235.00   151.57   0.23805E+04    0.22319E+04    0.0
 34     235.00   162.36   0.23429E+04    0.21863E+04    0.0
 35     235.00   174.26   0.23201E+04    0.21487E+04    0.0
 36     235.00   185.63   0.23087E+04    0.21259E+04    0.0
 37     235.00   195.50   0.22990E+04    0.21145E+04    0.0
 38     235.00   204.02   0.22809E+04    0.21048E+04    0.0
 39     235.00   212.23   0.22462E+04    0.20867E+04    0.0
 40     235.00   221.69   0.21925E+04    0.20520E+04    0.0
 41     235.00   229.39   0.21481E+04    0.32079E+04    0.0
 42     235.00   235.79   0.21146E+04    0.31635E+04    0.0
 43     235.00   240.97   0.20910E+04    0.31300E+04    0.0
 44     235.00   245.00   0.20749E+04    0.31064E+04    0.0
 45     235.00   248.03   0.20633E+04    0.30903E+04    0.0
 46     235.00   250.28   0.20545E+04    0.30787E+04    0.0
 47     235.00   251.95   0.20462E+04    0.30699E+04    0.0
 48     235.00   253.28   0.20367E+04    0.30616E+04    0.0
 49     235.00   254.50   0.20215E+04    0.30521E+04    0.0
 50     235.00   255.98   0.19846E+04    0.30369E+04    0.0
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```

```
  *** MATERIAL BALANCES ***



FEEDS

                          PLATE NO.  15
                   LB MOL/TIME     MOL FRAC
   ETHANE          0.37700E+02    0.92402E-02
   PROPANE         0.21561E+04    0.52846E+00
   IBUTANE         0.40050E+03    0.98162E-01
   NBUTANE         0.71530E+03    0.17532E+00
   IPENTANE        0.25120E+03    0.61569E-01
   NPENTANE        0.26710E+03    0.65466E-01
   HEXANE          0.14180E+03    0.34755E-01
   OCTANE          0.11030E+03    0.27034E-01
   TOTAL           0.40800E+04
```

```
CONNECTED STREAMS

                PLATE NO.  5  FROM 31
                LB MOL/TIME    MOL FRAC
   ETHANE       0.59456E+01   0.25785E-02
   PROPANE      0.19513E+04   0.84624E+00
   IBUTANE      0.25561E+03   0.11085E+00
   NBUTANE      0.92887E+02   0.40284E-01
   IPENTANE     0.73460E-01   0.31859E-04
   NPENTANE     0.97349E-02   0.42219E-05
   HEXANE       0.79791E-06   0.34604E-09
   OCTANE       0.55187E-13   0.23934E-16
   TOTAL        0.23058E+04

                PLATE NO. 25  FROM 50
                LB MOL/TIME    MOL FRAC
   ETHANE       0.17335E-04   0.87348E-08
   PROPANE      0.10793E+02   0.54382E-02
   IBUTANE      0.19609E+03   0.98808E-01
   NBUTANE      0.64466E+03   0.32483E+00
   IPENTANE     0.55735E+03   0.28084E+00
   NPENTANE     0.52583E+03   0.26496E+00
   HEXANE       0.44001E+02   0.22172E-01
   OCTANE       0.58530E+01   0.29492E-02
   TOTAL        0.19846E+04

                PLATE NO. 31  FROM  5
                LB MOL/TIME    MOL FRAC
   ETHANE       0.59507E+01   0.23803E-02
   PROPANE      0.19605E+04   0.78410E+00
   IBUTANE      0.36248E+03   0.14499E+00
   NBUTANE      0.17081E+03   0.68322E-01
   IPENTANE     0.25505E+00   0.10202E-03
   NPENTANE     0.42796E-01   0.17119E-04
   HEXANE       0.88358E-05   0.35343E-08
   OCTANE       0.27696E-11   0.11078E-14
   TOTAL        0.25000E+04

                PLATE NO. 50  FROM 25
                LB MOL/TIME    MOL FRAC
   ETHANE       0.14775E-03   0.49249E-07
   PROPANE      0.41388E+02   0.13796E-01
   IBUTANE      0.44574E+03   0.14858E+00
   NBUTANE      0.12523E+04   0.41742E+00
   IPENTANE     0.64633E+03   0.21544E+00
   NPENTANE     0.56440E+03   0.18813E+00
   HEXANE       0.44009E+02   0.14670E-01
   OCTANE       0.58526E+01   0.19509E-02
   TOTAL        0.30000E+04
```

```
PRODUCTS

                TOP PRODUCT ( 1)          BOTTOM PRODUCT (30)
          LB MOL/TIME   MOL FRAC     LB MOL/TIME   MOL FRAC
 ETHANE   0.37695E+02  0.17129E-01  0.65303E-09  0.97501E-12
 PROPANE  0.21164E+04  0.96174E+00  0.19924E-01  0.29748E-04
 IBUTANE  0.40011E+02  0.18182E-01  0.38486E+01  0.57462E-02
 NBUTANE  0.64387E+01  0.29258E-02  0.23299E+02  0.34786E-01
 IPENTANE 0.51366E-03  0.23342E-06  0.16202E+03  0.24191E+00
 NPENTANE 0.31892E-04  0.14492E-07  0.22848E+03  0.34114E+00
 HEXANE   0.11616E-09  0.52784E-13  0.14179E+03  0.21170E+00
 OCTANE   0.17576E-19  0.79868E-23  0.11030E+03  0.16468E+00
 TOTAL    0.22006E+04               0.66977E+03

                TOP PRODUCT (31)          BOTTOM PRODUCT (50)
          LB MOL/TIME   MOL FRAC     LB MOL/TIME   MOL FRAC
 ETHANE   0.59456E+01  0.25785E-02  0.17335E-04  0.87348E-08
 PROPANE  0.19513E+04  0.84624E+00  0.10793E+02  0.54382E-02
 IBUTANE  0.25561E+03  0.11085E+00  0.19609E+03  0.98808E-01
 NBUTANE  0.92887E+02  0.40284E-01  0.64466E+03  0.32483E+00
 IPENTANE 0.73460E-01  0.31859E-04  0.55735E+03  0.28084E+00
 NPENTANE 0.97349E-02  0.42219E-05  0.52583E+03  0.26496E+00
 HEXANE   0.79791E-06  0.34604E-09  0.44001E+02  0.22172E-01
 OCTANE   0.55187E-13  0.23934E-16  0.58530E+01  0.29492E-02
 TOTAL    0.23058E+04               0.19846E+04
```

```
LIQUID SIDE STREAMS

                      LIQUID ( 5)
               LB MOL/TIME     MOL FRAC
 ETHANE        0.59507E+01     0.23803E-02
 PROPANE       0.19605E+04     0.78419E+00
 IBUTANE       0.36248E+03     0.14499E+00
 NBUTANE       0.17081E+03     0.68322E-01
 IPENTANE      0.25505E+00     0.10202E-03
 NPENTANE      0.42796E-01     0.17119E-04
 HEXANE        0.88358E-05     0.35343E-08
 OCTANE        0.27696E-11     0.11078E-14
 TOTAL         0.25000E+04


VAPOUR SIDE STREAMS

                      VAPOUR (25)
               LB MOL/TIME     MOL FRAC
 ETHANE        0.14775E-03     0.49249E-07
 PROPANE       0.41388E+02     0.13796E-01
 IBUTANE       0.44574E+03     0.14858E+00
 NBUTANE       0.12523E+04     0.41742E+00
 IPENTANE      0.64633E+03     0.21544E+00
 NPENTANE      0.56440E+03     0.18813E+00
 HEXANE        0.44009E+02     0.14670E-01
 OCTANE        0.58526E+01     0.19509E-02
 TOTAL         0.30000E+04

                      VAPOUR (40)
               LB MOL/TIME     MOL FRAC
 ETHANE        0.91745E-04     0.75847E-07
 PROPANE       0.39612E+02     0.32748E-01
 IBUTANE       0.35667E+03     0.29486E+00
 NBUTANE       0.68555E+03     0.56676E+00
 IPENTANE      0.89136E+02     0.73690E-01
 NPENTANE      0.38597E+02     0.31909E-01
 HEXANE        0.93357E-02     0.77180E-05
 OCTANE        0.36103E-08     0.29847E-11
 TOTAL         0.12096E+04
```

```
  APPENDIX 6.2 -- EXTRACTIVE DISTILLATION SYSTEM

  ** PROBLEM STATEMENT **

       COLUMN NC 1 IS DISTILLATION COL.
NO OF PLATES= 17
COL PRESSURE      14.70 PSIA
PRESSURE DROP      0.0  PER PLATE
REBOILER VAPOUR     185.00 MOLES
REFLUX RATIO          3.000

       COLUMN NC 2 IS DISTILLATION COL.
NO OF PLATES= 20
COL PRESSURE      14.70 PSIA
PRESSURE DROP      0.0  PER PLATE
REBOILER VAPOUR     135.00 MOLES
REFLUX RATIO          2.000

       COLUMN NC 3 IS DISTILLATION COL.
NO OF PLATES=  5
COL PRESSURE      14.70 PSIA
PRESSURE DROP      0.0  PER PLATE
REBOILER VAPOUR      95.00 MOLES
REFLUX RATIO         10.000

 NO. OF FEEDS       1

    FEED 1 IS CN TO PLATE 11
      QUANTITY       0.10000E+03
      PRESSURE           14.70
      TEMP (F)          136.47
      ENTHALPY       0.31804E+06

 NO. OF INTERCCOLERS OR HEATERS      3

    INTERCOOLER OR HEATER 1 IS ON PLATE 17
      HEAT LOAD IS A VARIABLE

    INTERCOOLER OR HEATER 2 IS ON PLATE 37
      HEAT LOAD IS A VARIABLE

    INTERCOOLER OR HEATER 3 IS ON PLATE 42
      HEAT LOAD IS A VARIABLE


 *** STREAM CCNNECTIONS ***

    LEAVING    LEAVING   STREAM  ENTERING  ENTERING   ENTERING
    STREAM NO  STAGE NO  FLUID   FRACTION  STREAM NO  STAGE NO

        1         17       3       1.00       2          24
        2         37       3       1.00       3          40
        3         42       3       1.00       1           4

    STREAM FLUID   1=LIQUID SIDE STREAM  2=VAPOUR SIDE STREAM
                   3=LIQUID PRODUCT   4=VAPOUR PRODUCT
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

  0   SUM OF SQUARES OF RESIDUALS  0.14636E+02
     (MAT. BAL.  0.14605E+02   HEAT BAL.  0.31148E-01)
 TEMPERATURE (R)
  0.59360E+03 0.59460E+03 0.59560E+03 0.59660E+03 0.59760E+03
  0.59860E+03 0.59960E+03 0.60060E+03 0.60160E+03 0.60260E+03
  0.60360E+03 0.60460E+03 0.60560E+03 0.60660E+03 0.60760E+03
  0.60860E+03 0.60960E+03 0.59760E+03 0.60260E+03 0.60760E+03
  0.61260E+03 0.61760E+03 0.62260E+03 0.62560E+03 0.62760E+03
  0.62960E+03 0.63160E+03 0.63960E+03 0.63960E+03 0.63960E+03
  0.63960E+03 0.63960E+03 0.63960E+03 0.64460E+03 0.64960E+03
  0.65460E+03 0.65960E+03 0.60960E+03 0.63960E+03 0.65960E+03
  0.66460E+03 0.66960E+03
 VAPOUR FLOW RATE
  0.0         0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03
  0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03
  0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03
  0.20000E+03 0.18500E+03 0.0         0.16500E+03 0.16500E+03
  0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03
  0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03
  0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03
  0.16500E+03 0.13500E+03 0.0         0.11000E+03 0.11000E+03
  0.11000E+03 0.95000E+02

  1   SUM OF SQUARES OF RESIDUALS  0.26888E+02
     (MAT. BAL.  0.26868E+02   HEAT BAL.  0.20756E-01)
 TEMPERATURE (R)
  0.58860E+03 0.57241E+03 0.56798E+03 0.58905E+03 0.59540E+03
  0.59954E+03 0.60220E+03 0.60410E+03 0.60546E+03 0.60606E+03
  0.60504E+03 0.60591E+03 0.60678E+03 0.60768E+03 0.60872E+03
  0.61038E+03 0.61492E+03 0.59942E+03 0.60331E+03 0.60836E+03
  0.61393E+03 0.62014E+03 0.62685E+03 0.63234E+03 0.63719E+03
  0.64321E+03 0.65064E+03 0.66172E+03 0.66547E+03 0.66833E+03
  0.66960E+03 0.66883E+03 0.66602E+03 0.66367E+03 0.66040E+03
  0.65949E+03 0.66182E+03 0.61883E+03 0.64555E+03 0.66191E+03
  0.66575E+03 0.66976E+03
 VAPOUR FLOW RATE
  0.0         0.20898E+03 0.20448E+03 0.19320E+03 0.19110E+03
  0.19305E+03 0.19446E+03 0.19545E+03 0.19634E+03 0.19736E+03
  0.19885E+03 0.19845E+03 0.19849E+03 0.19850E+03 0.19844E+03
  0.19817E+03 0.18500E+03 0.0         0.16256E+03 0.16198E+03
  0.16126E+03 0.16027E+03 0.15927E+03 0.15828E+03 0.15975E+03
  0.16040E+03 0.16126E+03 0.16322E+03 0.16441E+03 0.16532E+03
  0.16617E+03 0.16673E+03 0.16679E+03 0.16674E+03 0.16495E+03
  0.16196E+03 0.13500E+03 0.0         0.10848E+03 0.10784E+03
  0.10761E+03 0.95000E+02
 2   SUM OF SQUARES OF RESIDUALS  0.12652E+02
   (MAT. BAL.  0.12640E+02   HEAT BAL.  0.11620E-01)
TEMPERATURE (R)
 0.58681E+03 0.56812E+03 0.50798E+03 0.53224E+03 0.55262E+03
 0.57342E+03 0.58770E+03 0.59704E+03 0.60290E+03 0.60578E+03
 0.60442E+03 0.60505E+03 0.60565E+03 0.60628E+03 0.60715E+03
 0.60924E+03 0.61767E+03 0.60194E+03 0.60591E+03 0.61171E+03
 0.61708E+03 0.62159E+03 0.62547E+03 0.63072E+03 0.63367E+03
 0.63696E+03 0.64167E+03 0.64903E+03 0.65100E+03 0.65289E+03
 0.65384E+03 0.65341E+03 0.65155E+03 0.65075E+03 0.65090E+03
 0.65513E+03 0.66144E+03 0.62463E+03 0.64486E+03 0.66216E+03
 0.66624E+03 0.66965E+03
VAPOUR FLOW RATE
 0.0         0.21603E+03 0.23357E+03 0.19962E+03 0.17356E+03
 0.17630E+03 0.18142E+03 0.18552E+03 0.18885E+03 0.19200E+03
 0.19598E+03 0.19599E+03 0.19607E+03 0.19609E+03 0.19595E+03
 0.19533E+03 0.18500E+03 0.0         0.15899E+03 0.15809E+03
 0.15739E+03 0.15633E+03 0.15502E+03 0.15270E+03 0.15483E+03
 0.15533E+03 0.15524E+03 0.15671E+03 0.15781E+03 0.15819E+03
 0.15877E+03 0.15923E+03 0.15935E+03 0.15885E+03 0.15641E+03
 0.15241E+03 0.13500E+03 0.0         0.10649E+03 0.10324E+03
 0.10329E+03 0.95000E+02

 3   SUM OF SQUARES OF RESIDUALS  0.63054E+01
   (MAT. BAL.  0.63004E+01   HEAT BAL.  0.49314E-02)
TEMPERATURE (R)
 0.58688E+03 0.57961E+03 0.56798E+03 0.58133E+03 0.58019E+03
 0.57967E+03 0.58540E+03 0.59304E+03 0.59970E+03 0.60388E+03
 0.60316E+03 0.60361E+03 0.60402E+03 0.60444E+03 0.60505E+03
 0.60694E+03 0.61686E+03 0.60220E+03 0.60543E+03 0.61092E+03
 0.61563E+03 0.61940E+03 0.62270E+03 0.62878E+03 0.63301E+03
 0.63728E+03 0.64181E+03 0.64716E+03 0.64791E+03 0.64833E+03
 0.64784E+03 0.64616E+03 0.64329E+03 0.64148E+03 0.64221E+03
 0.65001E+03 0.66038E+03 0.62706E+03 0.64156E+03 0.66127E+03
 0.66629E+03 0.66970E+03
VAPOUR FLOW RATE
 0.0         0.21743E+03 0.21095E+03 0.20217E+03 0.18761E+03
 0.18644E+03 0.18416E+03 0.18455E+03 0.18661E+03 0.18966E+03
 0.19434E+03 0.19481E+03 0.19489E+03 0.19492E+03 0.19479E+03
 0.19406E+03 0.18500E+03 0.0         0.15867E+03 0.15815E+03
 0.15795E+03 0.15676E+03 0.15467E+03 0.15107E+03 0.15368E+03
 0.15481E+03 0.15526E+03 0.15719E+03 0.15854E+03 0.15887E+03
 0.15920E+03 0.15934E+03 0.15912E+03 0.15801E+03 0.15440E+03
 0.14847E+03 0.13500E+03 0.0         0.10705E+03 0.10102E+03
 0.10094E+03 0.95000E+02
 4   SUM OF SQUARES OF RESIDUALS  0.49263E+00
    (MAT. BAL.  0.48590E+00   HEAT BAL.  0.67322E-02)
TEMPERATURE (R)
 0.58723E+03 0.59757E+03 0.60600E+03 0.60172E+03 0.59847E+03
 0.59641E+03 0.59377E+03 0.59352E+03 0.59663E+03 0.60077E+03
 0.60084E+03 0.60091E+03 0.60096E+03 0.60094E+03 0.60092E+03
 0.60185E+03 0.61354E+03 0.60213E+03 0.60364E+03 0.60855E+03
 0.61201E+03 0.61386E+03 0.61441E+03 0.62062E+03 0.62651E+03
 0.63213E+03 0.63733E+03 0.64029E+03 0.64079E+03 0.64036E+03
 0.63910E+03 0.63717E+03 0.63482E+03 0.63280E+03 0.63400E+03
 0.64539E+03 0.66131E+03 0.63948E+03 0.64513E+03 0.66385E+03
 0.66893E+03 0.67088E+03
VAPOUR FLOW RATE
 0.0         0.22069E+03 0.21558E+03 0.21269E+03 0.19152E+03
 0.18986E+03 0.18895E+03 0.18720E+03 0.18586E+03 0.18650E+03
 0.19086E+03 0.19197E+03 0.19204E+03 0.19213E+03 0.19217E+03
 0.19156E+03 0.18500E+03 0.0         0.15684E+03 0.15702E+03
 0.15793E+03 0.15696E+03 0.15384E+03 0.14750E+03 0.15003E+03
 0.15183E+03 0.15244E+03 0.15450E+03 0.15656E+03 0.15774E+03
 0.15886E+03 0.15983E+03 0.16053E+03 0.15997E+03 0.15556E+03
 0.14475E+03 0.13500E+03 0.0         0.11204E+03 0.98779E+02
 0.97134E+02 0.95000E+02

 5   SUM OF SQUARES OF RESIDUALS  0.45953E+00
    (MAT. BAL.  0.43940E+00   HEAT BAL.  0.20125E-01)
TEMPERATURE (R)
 0.58749E+03 0.59529E+03 0.59773E+03 0.60494E+03 0.60496E+03
 0.60491E+03 0.60460E+03 0.60378E+03 0.60279E+03 0.60281E+03
 0.60165E+03 0.60168E+03 0.60175E+03 0.60187E+03 0.60194E+03
 0.60201E+03 0.60984E+03 0.60199E+03 0.60357E+03 0.60807E+03
 0.61153E+03 0.61358E+03 0.61265E+03 0.61178E+03 0.61163E+03
 0.60947E+03 0.60968E+03 0.61290E+03 0.61713E+03 0.62186E+03
 0.62615E+03 0.62954E+03 0.63207E+03 0.63437E+03 0.63942E+03
 0.65202E+03 0.66539E+03 0.65044E+03 0.66263E+03 0.67055E+03
 0.67157E+03 0.67165E+03
VAPOUR FLOW RATE
 0.0         0.21256E+03 0.21134E+03 0.20404E+03 0.18901E+03
 0.18921E+03 0.18952E+03 0.18955E+03 0.18896E+03 0.18795E+03
 0.18945E+03 0.19002E+03 0.19003E+03 0.19014E+03 0.19043E+03
 0.19072E+03 0.18500E+03 0.0         0.16324E+03 0.16392E+03
 0.16521E+03 0.16486E+03 0.16214E+03 0.15669E+03 0.15902E+03
 0.16032E+03 0.15875E+03 0.15685E+03 0.15710E+03 0.15821E+03
 0.16038E+03 0.16332E+03 0.16659E+03 0.16870E+03 0.16633E+03
 0.15340E+03 0.13500E+03 0.0         0.12414E+03 0.10168E+03
 0.97202E+02 0.95000E+02
 6   SUM OF SQUARES OF RESIDUALS  0.34488E+00
   (MAT. BAL.  0.33790E+00   HEAT BAL.  0.69788E-02)
TEMPERATURE (R)
 0.58670E+03 0.59391E+03 0.59545E+03 0.60132E+03 0.60180E+03
 0.60234E+03 0.60271E+03 0.60283E+03 0.60282E+03 0.60304E+03
 0.60180E+03 0.60182E+03 0.60189E+03 0.60212E+03 0.60261E+03
 0.60357E+03 0.61107E+03 0.60296E+03 0.60427E+03 0.60817E+03
 0.61106E+03 0.61338E+03 0.61658E+03 0.62314E+03 0.63048E+03
 0.63653E+03 0.63967E+03 0.63904E+03 0.63633E+03 0.63272E+03
 0.62913E+03 0.62610E+03 0.62380E+03 0.62219E+03 0.62401E+03
 0.63985E+03 0.66132E+03 0.62588E+03 0.65006E+03 0.66785E+03
 0.67071E+03 0.67144E+03
VAPOUR FLOW RATE
 0.0         0.20961E+03 0.20902E+03 0.20225E+03 0.18533E+03
 0.18546E+03 0.18576E+03 0.18610E+03 0.18632E+03 0.18637E+03
 0.18813E+03 0.18872E+03 0.18870E+03 0.18870E+03 0.18883E+03
 0.18922E+03 0.18500E+03 0.0         0.17648E+03 0.17800E+03
 0.18048E+03 0.18178E+03 0.17894E+03 0.17134E+03 0.18024E+03
 0.18734E+03 0.19197E+03 0.19332E+03 0.19227E+03 0.19012E+03
 0.18793E+03 0.18627E+03 0.18518E+03 0.18366E+03 0.17592E+03
 0.15336E+03 0.13500E+03 0.0         0.95207E+02 0.92399E+02
 0.94294E+02 0.95000E+02

 7   SUM OF SQUARES OF RESIDUALS  0.11764E+00
   (MAT. BAL.  0.11673E+00   HEAT BAL.  0.91042E-03)
TEMPERATURE (R)
 0.58684E+03 0.59427E+03 0.59554E+03 0.60051E+03 0.60037E+03
 0.60041E+03 0.60063E+03 0.60095E+03 0.60132E+03 0.60184E+03
 0.60121E+03 0.60120E+03 0.60120E+03 0.60130E+03 0.60169E+03
 0.60280E+03 0.61026E+03 0.60067E+03 0.60268E+03 0.60832E+03
 0.61267E+03 0.61540E+03 0.61730E+03 0.62152E+03 0.62756E+03
 0.63204E+03 0.63463E+03 0.63565E+03 0.63613E+03 0.63660E+03
 0.63713E+03 0.63759E+03 0.63793E+03 0.63852E+03 0.64150E+03
 0.65171E+03 0.66503E+03 0.63388E+03 0.65852E+03 0.66879E+03
 0.67088E+03 0.67147E+03
VAPOUR FLOW RATE
 0.0         0.21193E+03 0.21088E+03 0.20382E+03 0.18632E+03
 0.18616E+03 0.18607E+03 0.18613E+03 0.18627E+03 0.18648E+03
 0.18822E+03 0.18904E+03 0.18903E+03 0.18899E+03 0.18896E+03
 0.18906E+03 0.18500E+03 0.0         0.15811E+03 0.15775E+03
 0.15926E+03 0.16108E+03 0.16128E+03 0.15676E+03 0.16215E+03
 0.16596E+03 0.16960E+03 0.17344E+03 0.17671E+03 0.17896E+03
 0.17994E+03 0.18098E+03 0.18183E+03 0.18190E+03 0.17792E+03
 0.15904E+03 0.13500E+03 0.0         0.10898E+03 0.96471E+02
 0.95200E+02 0.95000E+02
 8   SUM OF SQUARES OF RESIDUALS  0.76183E-01
   (MAT. BAL.  0.67220E-01   HEAT BAL.  0.89628E-02)
TEMPERATURE (R)
 0.58693E+03 0.59443E+03 0.59587E+03 0.60154E+03 0.60153E+03
 0.60150E+03 0.60153E+03 0.60165E+03 0.60186E+03 0.60220E+03
 0.60142E+03 0.60144E+03 0.60147E+03 0.60155E+03 0.60185E+03
 0.60285E+03 0.60998E+03 0.60145E+03 0.60477E+03 0.60903E+03
 0.61212E+03 0.61435E+03 0.61579E+03 0.61715E+03 0.62099E+03
 0.62349E+03 0.62494E+03 0.62582E+03 0.62665E+03 0.62781E+03
 0.62957E+03 0.63203E+03 0.63533E+03 0.63999E+03 0.64855E+03
 0.66160E+03 0.66944E+03 0.65122E+03 0.66844E+03 0.67112E+03
 0.67153E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21144E+03 0.21062E+03 0.20337E+03 0.18644E+03
 0.18644E+03 0.18641E+03 0.18638E+03 0.18641E+03 0.18655E+03
 0.18815E+03 0.18894E+03 0.18896E+03 0.18898E+03 0.18900E+03
 0.18902E+03 0.18500E+03 0.0         0.16384E+03 0.16352E+03
 0.16384E+03 0.16389E+03 0.16320E+03 0.15959E+03 0.16416E+03
 0.16765E+03 0.17012E+03 0.17200E+03 0.17317E+03 0.17367E+03
 0.17395E+03 0.17436E+03 0.17493E+03 0.17502E+03 0.17023E+03
 0.15225E+03 0.13500E+03 0.0         0.10766E+03 0.97172E+02
 0.95508E+02 0.95000E+02

 9   SUM OF SQUARES OF RESIDUALS  0.61316E-01
   (MAT. BAL.  0.60527E-01   HEAT BAL.  0.78889E-03)
TEMPERATURE (R)
 0.58687E+03 0.59432E+03 0.59572E+03 0.60125E+03 0.60131E+03
 0.60138E+03 0.60148E+03 0.60166E+03 0.60193E+03 0.60225E+03
 0.60144E+03 0.60145E+03 0.60150E+03 0.60161E+03 0.60196E+03
 0.60304E+03 0.61024E+03 0.60234E+03 0.60596E+03 0.61055E+03
 0.61397E+03 0.61619E+03 0.61774E+03 0.62098E+03 0.62647E+03
 0.62991E+03 0.63162E+03 0.63201E+03 0.63130E+03 0.62958E+03
 0.62706E+03 0.62447E+03 0.62363E+03 0.62765E+03 0.64033E+03
 0.65858E+03 0.66860E+03 0.64063E+03 0.66572E+03 0.67060E+03
 0.67138E+03 0.67158E+03
VAPOUR FLOW RATE
 0.0         0.21103E+03 0.21024E+03 0.20313E+03 0.18606E+03
 0.18609E+03 0.18611E+03 0.18614E+03 0.18620E+03 0.18640E+03
 0.18802E+03 0.18879E+03 0.18880E+03 0.18882E+03 0.18887E+03
 0.18891E+03 0.18500E+03 0.0         0.17860E+03 0.18007E+03
 0.18046E+03 0.17950E+03 0.17724E+03 0.17172E+03 0.17889E+03
 0.18422E+03 0.18769E+03 0.18968E+03 0.19057E+03 0.19051E+03
 0.18956E+03 0.18759E+03 0.18426E+03 0.17835E+03 0.16365E+03
 0.14159E+03 0.13500E+03 0.0         0.94717E+02 0.94555E+02
 0.94895E+02 0.95000E+02
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10    SUM OF SQUARES OF RESIDUALS  0.29587E-01
    (MAT. BAL.  0.29473E-01   HEAT BAL.  0.11421E-03)
TEMPERATURE (R)
 0.58687E+03 0.59433E+03 0.59571E+03 0.60115E+03 0.60117E+03
 0.60122E+03 0.60131E+03 0.60149E+03 0.60178E+03 0.60214E+03
 0.60138E+03 0.60139E+03 0.60142E+03 0.60153E+03 0.60186E+03
 0.60296E+03 0.61020E+03 0.60146E+03 0.60559E+03 0.61058E+03
 0.61397E+03 0.61609E+03 0.61754E+03 0.62030E+03 0.62541E+03
 0.62906E+03 0.63157E+03 0.63333E+03 0.63460E+03 0.63546E+03
 0.63594E+03 0.63600E+03 0.63549E+03 0.63558E+03 0.64325E+03
 0.65934E+03 0.66869E+03 0.64071E+03 0.66558E+03 0.67056E+03
 0.67137E+03 0.67158E+03
VAPOUR FLOW RATE
 0.0         0.21129E+03 0.21045E+03 0.20332E+03 0.18618E+03
 0.18618E+03 0.18618E+03 0.18620E+03 0.18625E+03 0.18645E+03
 0.18809E+03 0.18887E+03 0.18888E+03 0.18889E+03 0.18892E+03
 0.18893E+03 0.18500E+03 0.0         0.17107E+03 0.17263E+03
 0.17454E+03 0.17525E+03 0.17408E+03 0.16913E+03 0.17545E+03
 0.18012E+03 0.18348E+03 0.18580E+03 0.18755E+03 0.18910E+03
 0.19053E+03 0.19158E+03 0.19143E+03 0.18719E+03 0.16993E+03
 0.14451E+03 0.13500E+03 0.0         0.97957E+02 0.95086E+02
 0.95005E+02 0.95000E+02

11    SUM OF SQUARES OF RESIDUALS  0.18720E-01
    (MAT. BAL.  0.17724E-01   HEAT BAL.  0.99606E-03)
TEMPERATURE (R)
 0.58688E+03 0.59435E+03 0.59574E+03 0.60123E+03 0.60126E+03
 0.60131E+03 0.60139E+03 0.60155E+03 0.60183E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60187E+03
 0.60295E+03 0.61016E+03 0.60147E+03 0.60565E+03 0.61047E+03
 0.61386E+03 0.61599E+03 0.61735E+03 0.61956E+03 0.62373E+03
 0.62613E+03 0.62731E+03 0.62799E+03 0.62877E+03 0.62995E+03
 0.63151E+03 0.63316E+03 0.63490E+03 0.63866E+03 0.64952E+03
 0.66344E+03 0.66980E+03 0.65006E+03 0.66812E+03 0.67101E+03
 0.67148E+03 0.67161E+03
VAPOUR FLOW RATE
 0.0         0.21128E+03 0.21045E+03 0.20330E+03 0.18620E+03
 0.18621E+03 0.18622E+03 0.18623E+03 0.18627E+03 0.18647E+03
 0.18809E+03 0.18888E+03 0.18888E+03 0.18890E+03 0.18894E+03
 0.18894E+03 0.18500E+03 0.0         0.17067E+03 0.17143E+03
 0.17262E+03 0.17310E+03 0.17214E+03 0.16767E+03 0.17399E+03
 0.17827E+03 0.18078E+03 0.18188E+03 0.18224E+03 0.18244E+03
 0.18288E+03 0.18365E+03 0.18418E+03 0.18155E+03 0.16676E+03
 0.14445E+03 0.13500E+03 0.0         0.99206E+02 0.95499E+02
 0.95102E+02 0.95000E+02
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12   SUM OF SQUARES OF RESIDUALS  0.11358E-01
   (MAT. BAL.  0.11286E-01   HEAT BAL.  0.71254E-04)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60122E+03 0.60125E+03
 0.60130E+03 0.60139E+03 0.60156E+03 0.60183E+03 0.60218E+03
 0.60140E+03 0.60142E+03 0.60145E+03 0.60156E+03 0.60189E+03
 0.60297E+03 0.61018E+03 0.60176E+03 0.60607E+03 0.61081E+03
 0.61414E+03 0.61628E+03 0.61781E+03 0.62095E+03 0.62622E+03
 0.62954E+03 0.63120E+03 0.63162E+03 0.63117E+03 0.63020E+03
 0.62920E+03 0.62874E+03 0.62944E+03 0.63338E+03 0.64636E+03
 0.66250E+03 0.66962E+03 0.64761E+03 0.66761E+03 0.67093E+03
 0.67146E+03 0.67160E+03
VAPOUR FLOW RATE
 0.0         0.21123E+03 0.21041E+03 0.20327E+03 0.18617E+03
 0.18618E+03 0.18619E+03 0.18621E+03 0.18625E+03 0.18645E+03
 0.18808E+03 0.18886E+03 0.18886E+03 0.18888E+03 0.18892E+03
 0.18893E+03 0.18500E+03 0.0         0.17435E+03 0.17534E+03
 0.17633E+03 0.17646E+03 0.17517E+03 0.17028E+03 0.17746E+03
 0.18277E+03 0.18631E+03 0.18824E+03 0.18896E+03 0.18876E+03
 0.18792E+03 0.18673E+03 0.18495E+03 0.17910E+03 0.15961E+03
 0.13981E+03 0.13500E+03 0.0         0.96501E+02 0.94994E+02
 0.94994E+02 0.95000E+02

13   SUM OF SQUARES OF RESIDUALS  0.22546E-02
   (MAT. BAL.  0.21679E-02   HEAT BAL.  0.86734E-04)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60155E+03 0.60183E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60156E+03 0.60188E+03
 0.60296E+03 0.61018E+03 0.60168E+03 0.60598E+03 0.61075E+03
 0.61408E+03 0.61619E+03 0.61765E+03 0.62051E+03 0.62567E+03
 0.62910E+03 0.63110E+03 0.63207E+03 0.63234E+03 0.63214E+03
 0.63179E+03 0.63166E+03 0.63243E+03 0.63660E+03 0.64942E+03
 0.66391E+03 0.66995E+03 0.65109E+03 0.66831E+03 0.67105E+03
 0.67149E+03 0.67161E+03
VAPOUR FLOW RATE
 0.0         0.21124E+03 0.21042E+03 0.20328E+03 0.18618E+03
 0.18618E+03 0.18619E+03 0.18621E+03 0.18625E+03 0.18645E+03
 0.18808E+03 0.18886E+03 0.18887E+03 0.18888E+03 0.18892E+03
 0.18893E+03 0.18500E+03 0.0         0.17314E+03 0.17418E+03
 0.17524E+03 0.17543E+03 0.17419E+03 0.16941E+03 0.17615E+03
 0.18113E+03 0.18455E+03 0.18663E+03 0.18778E+03 0.18826E+03
 0.18821E+03 0.18771E+03 0.18627E+03 0.18033E+03 0.16069E+03
 0.14062E+03 0.13500E+03 0.0         0.97044E+02 0.95137E+02
 0.95025E+02 0.95000E+02
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14    SUM OF SQUARES OF RESIDUALS  0.21157E-02
    (MAT. BAL.  0.19336E-02   HEAT BAL.  0.18207E-03)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60155E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61018E+03 0.60168E+03 0.60599E+03 0.61076E+03
 0.61408E+03 0.61616E+03 0.61757E+03 0.62020E+03 0.62513E+03
 0.62839E+03 0.63035E+03 0.63144E+03 0.63199E+03 0.63218E+03
 0.63221E+03 0.63239E+03 0.63347E+03 0.63825E+03 0.65143E+03
 0.66488E+03 0.67018E+03 0.65371E+03 0.66878E+03 0.67114E+03
 0.67152E+03 0.67161E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20328E+03 0.18618E+03
 0.18618E+03 0.18619E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18888E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17296E+03 0.17403E+03
 0.17513E+03 0.17530E+03 0.17404E+03 0.16930E+03 0.17584E+03
 0.18059E+03 0.18379E+03 0.18572E+03 0.18686E+03 0.18749E+03
 0.18772E+03 0.18751E+03 0.18618E+03 0.17980E+03 0.15968E+03
 0.14039E+03 0.13500E+03 0.0         0.97055E+02 0.95168E+02
 0.95032E+02 0.95000E+02

15    SUM OF SQUARES OF RESIDUALS  0.78507E-03
    (MAT. BAL.  0.74456E-03   HEAT BAL.  0.40508E-04)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61018E+03 0.60174E+03 0.60609E+03 0.61085E+03
 0.61415E+03 0.61621E+03 0.61758E+03 0.62008E+03 0.62480E+03
 0.62779E+03 0.62947E+03 0.63039E+03 0.63091E+03 0.63121E+03
 0.63136E+03 0.63155E+03 0.63257E+03 0.63775E+03 0.65203E+03
 0.66537E+03 0.67031E+03 0.65522E+03 0.66903E+03 0.67118E+03
 0.67153E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21043E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18620E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17363E+03 0.17480E+03
 0.17594E+03 0.17611E+03 0.17477E+03 0.16998E+03 0.17653E+03
 0.18116E+03 0.18413E+03 0.18580E+03 0.18670E+03 0.18722E+03
 0.18748E+03 0.18733E+03 0.18578E+03 0.17784E+03 0.15596E+03
 0.13889E+03 0.13500E+03 0.0         0.96498E+02 0.95084E+02
 0.95015E+02 0.95000E+02
```

```
16   SUM OF SQUARES OF RESIDUALS  0.46230E-03
   (MAT. BAL.  0.45865E-03   HEAT BAL.  0.36572E-05)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61018E+03 0.60176E+03 0.60610E+03 0.61087E+03
 0.61418E+03 0.61625E+03 0.61765E+03 0.62026E+03 0.62507E+03
 0.62813E+03 0.62984E+03 0.63072E+03 0.63116E+03 0.63135E+03
 0.63134E+03 0.63126E+03 0.63177E+03 0.63631E+03 0.65092E+03
 0.66499E+03 0.67023E+03 0.65415E+03 0.66885E+03 0.67116E+03
 0.67152E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18620E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17389E+03 0.17507E+03
 0.17626E+03 0.17646E+03 0.17513E+03 0.17029E+03 0.17695E+03
 0.18169E+03 0.18475E+03 0.18647E+03 0.18737E+03 0.18785E+03
 0.18807E+03 0.18791E+03 0.18630E+03 0.17782E+03 0.15507E+03
 0.13839E+03 0.13500E+03 0.0         0.96275E+02 0.95036E+02
 0.95005E+02 0.95000E+02

17   SUM OF SQUARES OF RESIDUALS  0.25302E-03
   (MAT. BAL.  0.25201E-03   HEAT BAL.  0.10123E-05)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61017E+03 0.60174E+03 0.60608E+03 0.61087E+03
 0.61419E+03 0.61628E+03 0.61769E+03 0.62037E+03 0.62526E+03
 0.62843E+03 0.63023E+03 0.63121E+03 0.63174E+03 0.63203E+03
 0.63217E+03 0.63219E+03 0.63257E+03 0.63662E+03 0.65093E+03
 0.66496E+03 0.67022E+03 0.65405E+03 0.66884E+03 0.67115E+03
 0.67152E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18620E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17370E+03 0.17486E+03
 0.17608E+03 0.17635E+03 0.17507E+03 0.17024E+03 0.17693E+03
 0.18172E+03 0.18486E+03 0.18666E+03 0.18762E+03 0.18815E+03
 0.18847E+03 0.18852E+03 0.18725E+03 0.17889E+03 0.15557E+03
 0.13849E+03 0.13500E+03 0.0         0.96303E+02 0.95039E+02
 0.95005E+02 0.95000E+02
```

```
18   SUM OF SQUARES OF RESIDUALS  0.30540E-03
   (MAT. BAL.  0.29455E-03   HEAT BAL.  0.10846E-04)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61017E+03 0.60173E+03 0.60607E+03 0.61086E+03
 0.61418E+03 0.61626E+03 0.61766E+03 0.62030E+03 0.62514E+03
 0.62826E+03 0.63004E+03 0.63099E+03 0.63152E+03 0.63185E+03
 0.63210E+03 0.63234E+03 0.63305E+03 0.63753E+03 0.65182E+03
 0.66532E+03 0.67030E+03 0.65507E+03 0.66901E+03 0.67118E+03
 0.67153E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18619E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17354E+03 0.17468E+03
 0.17587E+03 0.17613E+03 0.17487E+03 0.17007E+03 0.17672E+03
 0.18146E+03 0.18456E+03 0.18633E+03 0.18726E+03 0.18774E+03
 0.18803E+03 0.18808E+03 0.18690E+03 0.17872E+03 0.15567E+03
 0.13866E+03 0.13500E+03 0.0         0.96402E+02 0.95066E+02
 0.95011E+02 0.95000E+02

19   SUM OF SQUARES OF RESIDUALS  0.20242E-03
   (MAT. BAL.  0.18517E-03   HEAT BAL.  0.17249E-04)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61017E+03 0.60175E+03 0.60610E+03 0.61087E+03
 0.61418E+03 0.61626E+03 0.61766E+03 0.62027E+03 0.62509E+03
 0.62817E+03 0.62989E+03 0.63077E+03 0.63119E+03 0.63142E+03
 0.63161E+03 0.63193E+03 0.63293E+03 0.63795E+03 0.65258E+03
 0.66568E+03 0.67038E+03 0.65614E+03 0.66918E+03 0.67121E+03
 0.67153E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18619E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17364E+03 0.17476E+03
 0.17592E+03 0.17614E+03 0.17487E+03 0.17008E+03 0.17673E+03
 0.18146E+03 0.18455E+03 0.18629E+03 0.18717E+03 0.18757E+03
 0.18771E+03 0.18760E+03 0.18625E+03 0.17774E+03 0.15470E+03
 0.13841E+03 0.13500E+03 0.0         0.96340E+02 0.95065E+02
 0.95011E+02 0.95000E+02
```

```
20    SUM OF SQUARES OF RESIDUALS  0.69671E-04
    (MAT. BAL.  0.68904E-04   HEAT BAL.  0.76733E-06)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59573E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61017E+03 0.60177E+03 0.60612E+03 0.61090E+03
 0.61420E+03 0.61628E+03 0.61768E+03 0.62032E+03 0.62519E+03
 0.62833E+03 0.63010E+03 0.63102E+03 0.63143E+03 0.63157E+03
 0.63158E+03 0.63163E+03 0.63237E+03 0.63735E+03 0.65238E+03
 0.66566E+03 0.67039E+03 0.65614E+03 0.66918E+03 0.67121E+03
 0.67153E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18619E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17386E+03 0.17501E+03
 0.17617E+03 0.17658E+03 0.17509E+03 0.17027E+03 0.17695E+03
 0.18172E+03 0.18484E+03 0.18664E+03 0.18760E+03 0.18806E+03
 0.18820E+03 0.18797E+03 0.18633E+03 0.17710E+03 0.15354E+03
 0.13796E+03 0.13500E+03 0.0         0.96168E+02 0.95036E+02
 0.95006E+02 0.95000E+02

21    SUM OF SQUARES OF RESIDUALS  0.15176E-04
    (MAT. BAL.  0.14273E-04   HEAT BAL.  0.90351E-06)
TEMPERATURE (R)
 0.58687E+03 0.59434E+03 0.59572E+03 0.60121E+03 0.60124E+03
 0.60129E+03 0.60138E+03 0.60154E+03 0.60182E+03 0.60217E+03
 0.60140E+03 0.60141E+03 0.60145E+03 0.60155E+03 0.60188E+03
 0.60296E+03 0.61017E+03 0.60176E+03 0.60612E+03 0.61089E+03
 0.61420E+03 0.61628E+03 0.61767E+03 0.62030E+03 0.62515E+03
 0.62828E+03 0.63007E+03 0.63102E+03 0.63150E+03 0.63172E+03
 0.63179E+03 0.63189E+03 0.63263E+03 0.63760E+03 0.65259E+03
 0.66574E+03 0.67040E+03 0.65637E+03 0.66921E+03 0.67122E+03
 0.67154E+03 0.67162E+03
VAPOUR FLOW RATE
 0.0         0.21125E+03 0.21042E+03 0.20329E+03 0.18618E+03
 0.18619E+03 0.18619E+03 0.18621E+03 0.18626E+03 0.18646E+03
 0.18808E+03 0.18887E+03 0.18887E+03 0.18889E+03 0.18893E+03
 0.18893E+03 0.18500E+03 0.0         0.17380E+03 0.17495E+03
 0.17612E+03 0.17634E+03 0.17505E+03 0.17024E+03 0.17690E+03
 0.18164E+03 0.18475E+03 0.18654E+03 0.18751E+03 0.18801E+03
 0.18822E+03 0.18808E+03 0.18650E+03 0.17724E+03 0.15360E+03
 0.13800E+03 0.13500E+03 0.0         0.96187E+02 0.95041E+02
 0.95007E+02 0.95000E+02
```

```
     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS  21

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 1    14.70 PSIA   136.47 F    0.31804E+06 BTU    1.000

*** STREAM CONNECTIONS ***

LEAVING     LEAVING    STREAM   ENTERING  ENTERING    ENTERING
STREAM NO   STAGE NO   FLUID    FRACTION  STREAM NO   STAGE NO

     1          17        3        1.00        2           24
     2          37        3        1.00        3           40
     3          42        3        1.00        1            4

STREAM FLUID   1=LIQUID SIDE STREAM  2=VAPOUR SIDE STREAM
               3=LIQUID PRODUCT  4=VAPOUR PRODUCT
```

```
*** STAGE VARIABLES ***

 PLATE  PRESSURE   TEMP     LIQUID FLOW    VAPOUR FLOW    HEAT DUTY
  NO      PSIA       F      LB MOL/TIME    LB MOL/TIME    BTU/TIME
   1      14.70   127.27    0.15844E+03    0.0           -0.27822E+07
   2      14.70   134.74    0.15761E+03    0.21125E+03    0.0
   3      14.70   136.13    0.15047E+03    0.21042E+03    0.0
   4      14.70   141.61    0.33338E+03    0.20329E+03    0.0
   5      14.70   141.64    0.33338E+03    0.18618E+03    0.0
   6      14.70   141.69    0.33339E+03    0.18619E+03    0.0
   7      14.70   141.78    0.33341E+03    0.18619E+03    0.0
   8      14.70   141.94    0.33345E+03    0.18621E+03    0.0
   9      14.70   142.22    0.33365E+03    0.18626E+03    0.0
  10      14.70   142.57    0.33528E+03    0.18646E+03    0.0
  11      14.70   141.80    0.43606E+03    0.18808E+03    0.0
  12      14.70   141.81    0.43607E+03    0.18887E+03    0.0
  13      14.70   141.85    0.43608E+03    0.18887E+03    0.0
  14      14.70   141.95    0.43612E+03    0.18889E+03    0.0
  15      14.70   142.28    0.43613E+03    0.18893E+03    0.0
  16      14.70   143.36    0.43220E+03    0.18893E+03    0.0
  17      14.70   150.57    0.24720E+03    0.18500E+03    0.25664E+07
  ---------------------------------------------------------------------
  18      14.70   142.16    0.11587E+03    0.0           -0.22112E+07
  19      14.70   146.52    0.11702E+03    0.17380E+03    0.0
  20      14.70   151.29    0.11819E+03    0.17495E+03    0.0
  21      14.70   154.60    0.11841E+03    0.17612E+03    0.0
  22      14.70   156.68    0.11712E+03    0.17634E+03    0.0
  23      14.70   158.07    0.11230E+03    0.17505E+03    0.0
  24      14.70   160.70    0.36616E+03    0.17024E+03    0.0
  25      14.70   165.55    0.37090E+03    0.17690E+03    0.0
  26      14.70   168.68    0.37401E+03    0.18164E+03    0.0
  27      14.70   170.47    0.37580E+03    0.18475E+03    0.0
  28      14.70   171.42    0.37677E+03    0.18654E+03    0.0
  29      14.70   171.90    0.37727E+03    0.18751E+03    0.0
  30      14.70   172.12    0.37748E+03    0.18801E+03    0.0
  31      14.70   172.19    0.37735E+03    0.18822E+03    0.0
  32      14.70   172.29    0.37577E+03    0.18808E+03    0.0
  33      14.70   173.03    0.36651E+03    0.18650E+03    0.0
  34      14.70   178.00    0.34286E+03    0.17724E+03    0.0
  35      14.70   192.99    0.32726E+03    0.15360E+03    0.0
  36      14.70   206.14    0.32426E+03    0.13800E+03    0.0
  37      14.70   210.80    0.18926E+03    0.13500E+03    0.24025E+07
  ---------------------------------------------------------------------
  38      14.70   196.77    0.87442E+02    0.0           -0.16930E+07
  39      14.70   209.61    0.86297E+02    0.96187E+02    0.0
  40      14.70   211.62    0.27552E+03    0.95041E+02    0.0
  41      14.70   211.94    0.27552E+03    0.95007E+02    0.0
  42      14.70   212.02    0.18052E+03    0.95000E+02    0.16947E+07
  ---------------------------------------------------------------------
```

```
*** MATERIAL BALANCES ***


FEEDS

                        PLATE NO.  11
             LB MOL/TIME      MOL FRAC
ACETONE      0.90000E+02    0.90000E+00
ANITRILE     0.10000E+02    0.10000E+00
WATER        0.0            0.0
TOTAL        0.10000E+03


 CONNECTED STREAMS

             PLATE NO.   4  FROM 42
             LB MOL/TIME      MOL FRAC
ACETONE      0.18317E-07    0.91580E-10
ANITRILE     0.81576E-02    0.40786E-04
WATER        0.20000E+03    0.99996E+00
TOTAL        0.20001E+03

MAKEUP OF WATER       0.19491E+02

             PLATE NO. 24   FROM 17
             LB MOL/TIME      MOL FRAC
ACETONE      0.41165E+02    0.16653E+00
ANITRILE     0.10003E+02    0.40468E-01
WATER        0.19603E+03    0.79300E+00
TOTAL        0.24720E+03

             PLATE NO. 40   FROM 37
             LB MOL/TIME      MOL FRAC
ACETONE      0.15396E-04    0.81350E-07
ANITRILE     0.46185E+00    0.24403E-02
WATER        0.18880E+03    0.99756E+00
TOTAL        0.18926E+03
```

```
PRODUCTS

                 TOP PRODUCT ( 1)            BOTTOM PRODUCT (17)
            LB MOL/TIME    MOL FRAC     LB MOL/TIME    MOL FRAC
ACETONE     0.48835E+02   0.92467E+00   0.41165E+02   0.16653E+00
ANITRILE    0.47907E-02   0.90710E-04   0.10003E+02   0.40468E-01
WATER       0.39737E+01   0.75241E-01   0.19603E+03   0.79300E+00
TOTAL       0.52813E+02                 0.24720E+03

                 TOP PRODUCT (18)            BOTTOM PRODUCT (37)
            LB MOL/TIME    MOL FRAC     LB MOL/TIME    MOL FRAC
ACETONE     0.41165E+02   0.71056E+00   0.15396E-04   0.81350E-07
ANITRILE    0.95416E+01   0.16470E+00   0.46185E+00   0.24403E-02
WATER       0.72265E+01   0.12474E+00   0.18880E+03   0.99756E+00
TOTAL       0.57933E+02                 0.18926E+03

                 TOP PRODUCT (38)            BOTTOM PRODUCT (42)
            LB MOL/TIME    MOL FRAC     LB MOL/TIME    MOL FRAC
ACETONE     0.15378E-04   0.17586E-05   0.18315E-07   0.10146E-09
ANITRILE    0.45369E+00   0.51884E-01   0.81568E-02   0.45186E-04
WATER       0.82905E+01   0.94811E+00   0.18051E+03   0.99995E+00
TOTAL       0.87442E+01                 0.18052E+03
```

```
APPENDIX 6.3 -- AMINE TREATING SYSTEM

    ** PROBLEM STATEMENT **

       COLUMN NO 1 IS CONTACTOR
NO OF PLATES= 10
COL PRESSURE     250.00 PSIA
PRESSURE DROP      0.0  PER PLATE

       COLUMN NO 2 IS REGENERATOR
NO OF PLATES= 14
CONDENSER TEMPERATURE     120.00 (F)
             PRESSURE      27.00 PSIA
COL PRESSURE      28.00 PSIA
PRESSURE DROP      0.33 PER PLATE

 NO. OF FEEDS       1

   FEED 1 IS ON TO PLATE 10
     QUANTITY       0.13158E+05
     PRESSURE          250.00
     TEMP (F)           90.00
     ENTHALPY       0.84300E+08

 NO. OF LIQUID SIDE STREAMS       1

   STREAM 1 LEAVES PLATE 17
     QUANTITY       0.25500E+04

 NO. OF INTERCOOLERS OR HEATERS       2

   INTERCOOLER OR HEATER 1 IS ON PLATE 11
     HEAT LOAD IS A VARIABLE

   INTERCOOLER OR HEATER 2 IS ON PLATE 24
     HEAT LOAD (BTU/TIME)       0.13800E+08


  *** STREAM CONNECTIONS ***

   LEAVING     LEAVING     STREAM  ENTERING     ENTERING
   STREAM NO.  STAGE NO.   FLUID   STREAM NO.   STAGE NO.

       1          10         3         3           12
       2          17         1         2            5
       3          24         3         1            1

 ENTERING TEMPS (F) - SEMILEAN  100.00
                          RICH  190.00
                          LEAN  110.00

 AMINE IN LEAN AMINE STREAM    127.350 MOLES/TIME
 SOLUTION STRENGTH (WT PCT)     15.30
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0   SUM OF SQUARES OF RESIDUALS  0.16212E+00
    (MAT. BAL.  0.15918E+00   HEAT BAL.  0.29369E-02)
TEMPERATURE (R)
 0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03
 0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03 0.56960E+03
 0.57960E+03 0.68960E+03 0.69160E+03 0.69360E+03 0.69560E+03
 0.69760E+03 0.69960E+03 0.70160E+03 0.70360E+03 0.70560E+03
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03
VAPOUR FLOW RATE
 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05
 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05
 0.80000E+02 0.24000E+03 0.50000E+03 0.60000E+03 0.61500E+03
 0.63000E+03 0.64500E+03 0.66000E+03 0.67500E+03 0.69000E+03
 0.70500E+03 0.72000E+03 0.73500E+03 0.75000E+03

 1   SUM OF SQUARES OF RESIDUALS  0.18974E-01
    (MAT. BAL.  0.18321E-01   HEAT BAL.  0.65241E-03)
TEMPERATURE (R)
 0.56069E+03 0.55928E+03 0.55877E+03 0.55859E+03 0.55853E+03
 0.55807E+03 0.55775E+03 0.55752E+03 0.55734E+03 0.56129E+03
 0.57960E+03 0.69281E+03 0.69858E+03 0.70159E+03 0.70388E+03
 0.70547E+03 0.70672E+03 0.70784E+03 0.70901E+03 0.71004E+03
 0.71109E+03 0.71220E+03 0.71338E+03 0.71496E+03
VAPOUR FLOW RATE
 0.13109E+05 0.13107E+05 0.13106E+05 0.13106E+05 0.13106E+05
 0.13106E+05 0.13105E+05 0.13105E+05 0.13105E+05 0.13105E+05
 0.81395E+02 0.29302E+03 0.60380E+03 0.68485E+03 0.70365E+03
 0.71762E+03 0.72700E+03 0.73457E+03 0.75207E+03 0.75385E+03
 0.75673E+03 0.76124E+03 0.76759E+03 0.77405E+03

 2   SUM OF SQUARES OF RESIDUALS  0.48659E-02
    (MAT. BAL.  0.42469E-02   HEAT BAL.  0.61894E-03)
TEMPERATURE (R)
 0.56243E+03 0.55989E+03 0.55912E+03 0.55889E+03 0.55881E+03
 0.55858E+03 0.55851E+03 0.55853E+03 0.55851E+03 0.55744E+03
 0.57960E+03 0.69551E+03 0.70446E+03 0.70700E+03 0.70836E+03
 0.70939E+03 0.71043E+03 0.71163E+03 0.71231E+03 0.71300E+03
 0.71366E+03 0.71430E+03 0.71493E+03 0.71621E+03
VAPOUR FLOW RATE
 0.13128E+05 0.13125E+05 0.13124E+05 0.13124E+05 0.13124E+05
 0.13124E+05 0.13124E+05 0.13124E+05 0.13125E+05 0.13132E+05
 0.82190E+02 0.36893E+03 0.67243E+03 0.73334E+03 0.75346E+03
 0.76524E+03 0.79608E+03 0.79948E+03 0.79447E+03 0.79489E+03
 0.79545E+03 0.79681E+03 0.79927E+03 0.80175E+03
 3   SUM OF SQUARES OF RESIDUALS  0.41652E-02
    (MAT. BAL.  0.36962E-02   HEAT BAL.  0.46896E-03)
TEMPERATURE (R)
 0.56362E+03 0.56168E+03 0.56112E+03 0.56096E+03 0.56087E+03
 0.56130E+03 0.56160E+03 0.56180E+03 0.56183E+03 0.56094E+03
 0.57960E+03 0.69196E+03 0.70130E+03 0.70491E+03 0.70783E+03
 0.70938E+03 0.71051E+03 0.71145E+03 0.71221E+03 0.71292E+03
 0.71360E+03 0.71426E+03 0.71492E+03 0.71619E+03
VAPOUR FLOW RATE
 0.13130E+05 0.13128E+05 0.13127E+05 0.13127E+05 0.13127E+05
 0.13128E+05 0.13129E+05 0.13129E+05 0.13129E+05 0.13138E+05
 0.80818E+02 0.28280E+03 0.59897E+03 0.70839E+03 0.73649E+03
 0.76015E+03 0.76232E+03 0.78054E+03 0.78753E+03 0.79182E+03
 0.79563E+03 0.79928E+03 0.80290E+03 0.80628E+03

 4   SUM OF SQUARES OF RESIDUALS  0.16528E-02
    (MAT. BAL.  0.14852E-02   HEAT BAL.  0.16760E-03)
TEMPERATURE (R)
 0.56350E+03 0.56189E+03 0.56139E+03 0.56123E+03 0.56112E+03
 0.56156E+03 0.56183E+03 0.56200E+03 0.56204E+03 0.56039E+03
 0.57960E+03 0.69373E+03 0.70275E+03 0.70588E+03 0.70824E+03
 0.70959E+03 0.71058E+03 0.71146E+03 0.71221E+03 0.71290E+03
 0.71357E+03 0.71422E+03 0.71488E+03 0.71617E+03
VAPOUR FLOW RATE
 0.13130E+05 0.13128E+05 0.13128E+05 0.13127E+05 0.13127E+05
 0.13129E+05 0.13129E+05 0.13130E+05 0.13130E+05 0.13138E+05
 0.80739E+02 0.32932E+03 0.62176E+03 0.68141E+03 0.72657E+03
 0.75480E+03 0.77300E+03 0.78439E+03 0.78986E+03 0.79408E+03
 0.79775E+03 0.80112E+03 0.80436E+03 0.80666E+03

 5   SUM OF SQUARES OF RESIDUALS  0.43916E-04
    (MAT. BAL.  0.33733E-04   HEAT BAL.  0.10183E-04)
TEMPERATURE (R)
 0.56350E+03 0.56186E+03 0.56136E+03 0.56120E+03 0.56111E+03
 0.56153E+03 0.56179E+03 0.56194E+03 0.56196E+03 0.56035E+03
 0.57960E+03 0.69271E+03 0.70197E+03 0.70542E+03 0.70800E+03
 0.70942E+03 0.71047E+03 0.71139E+03 0.71215E+03 0.71285E+03
 0.71353E+03 0.71419E+03 0.71486E+03 0.71616E+03
VAPOUR FLOW RATE
 0.13130E+05 0.13128E+05 0.13127E+05 0.13127E+05 0.13127E+05
 0.13129E+05 0.13129E+05 0.13129E+05 0.13130E+05 0.13138E+05
 0.81278E+02 0.31311E+03 0.60975E+03 0.68465E+03 0.72837E+03
 0.75686E+03 0.77352E+03 0.78477E+03 0.79017E+03 0.79428E+03
 0.79782E+03 0.80108E+03 0.80409E+03 0.80639E+03
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  6   SUM OF SQUARES OF RESIDUALS  0.20399E-04
     (MAT. BAL.  0.15996E-04   HEAT BAL.  0.44027E-05)
 TEMPERATURE (R)
  0.56363E+03 0.56187E+03 0.56133E+03 0.56117E+03 0.56108E+03
  0.56148E+03 0.56172E+03 0.56186E+03 0.56185E+03 0.56026E+03
  0.57960E+03 0.69218E+03 0.70159E+03 0.70527E+03 0.70793E+03
  0.70938E+03 0.71045E+03 0.71137E+03 0.71214E+03 0.71285E+03
  0.71353E+03 0.71420E+03 0.71487E+03 0.71617E+03
 VAPOUR FLOW RATE
  0.13130E+05 0.13128E+05 0.13127E+05 0.13127E+05 0.13127E+05
  0.13129E+05 0.13129E+05 0.13129E+05 0.13130E+05 0.13138E+05
  0.82221E+02 0.31078E+03 0.60555E+03 0.69001E+03 0.73152E+03
  0.75864E+03 0.77355E+03 0.78451E+03 0.78976E+03 0.79371E+03
  0.79711E+03 0.80023E+03 0.80322E+03 0.80580E+03
 ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS   6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.25000E+03 PSIA    0.90000E+02 F     0.84300E+08 B.T.U.       0.0


*** STREAM CONNECTIONS ***

   LEAVING      LEAVING    STREAM  ENTERING     ENTERING
   STREAM NO.   STAGE NO.  FLUID   STREAM NO.   STAGE NO.

       1           10        3        3            12
       2           17        1        2             5
       3           24        3        1             1

   STREAM FLUID  1=LIQUID SIDE STREAM  3=LIQUID PRODUCT


*** STAGE VARIABLES ***

PLATE  PRESSURE  TEMP   LIQUID FLOW   VAPOUR FLOW   HEAT DUTY
 NO      PSIA     F     LB MOL/TIME   LB MOL/TIME   BTU/TIME
  1     250.00  104.03  0.25214E+04   0.13130E+05   0.0
  2     250.00  102.27  0.25206E+04   0.13128E+05   0.0
  3     250.00  101.73  0.25204E+04   0.13127E+05   0.0
  4     250.00  101.57  0.25206E+04   0.13127E+05   0.0
  5     250.00  101.48  0.50719E+04   0.13127E+05   0.0
  6     250.00  101.88  0.50722E+04   0.13129E+05   0.0
  7     250.00  102.12  0.50725E+04   0.13129E+05   0.0
  8     250.00  102.26  0.50730E+04   0.13129E+05   0.0
  9     250.00  102.25  0.50813E+04   0.13130E+05   0.0
 10     250.00  100.66  0.51013E+04   0.13138E+05   0.0
 ------------------------------------------------------------
 11      27.00  120.00  0.22856E+03   0.82221E+02 -0.45829E+07
 12      28.00  232.58  0.56247E+04   0.31078E+03   0.0
 13      28.33  241.99  0.57091E+04   0.60555E+03   0.0
 14      28.67  245.67  0.57506E+04   0.69001E+03   0.0
 15      29.00  248.33  0.57778E+04   0.73152E+03   0.0
 16      29.33  249.78  0.57927E+04   0.75864E+03   0.0
 17      29.67  250.85  0.32536E+04   0.77355E+03   0.0
 18      30.00  251.77  0.32589E+04   0.78451E+03   0.0
 19      30.33  252.54  0.32628E+04   0.78976E+03   0.0
 20      30.67  253.25  0.32662E+04   0.79371E+03   0.0
 21      31.00  253.93  0.32693E+04   0.79711E+03   0.0
 22      31.33  254.60  0.32723E+04   0.80023E+03   0.0
 23      31.67  255.27  0.32749E+04   0.80322E+03   0.0
 24      32.00  256.57  0.24691E+04   0.80580E+03   0.13800E+08
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REFLUX RATIO FOR REGENERATOR =  2.780
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*** MATERIAL BALANCES ***

SOUR GAS FEED

                  PLATE NO.   10
               LB MOL/TIME      MOL FRAC
 H2S           0.35700E+02    0.27131E-02
 CO2           0.39500E+02    0.30019E-02
 MEA           0.0            0.0
 WATER         0.50000E+01    0.37999E-03
 HYDROGEN      0.50000E+03    0.37999E-01
 NITROGEN      0.50000E+04    0.37999E+00
 METHANE       0.40000E+04    0.30399E+00
 ETHANE        0.25000E+04    0.19000E+00
 PROPANE       0.90000E+03    0.68398E-01
 N-BUTANE      0.89000E+02    0.67638E-02
 I-BUTANE      0.89000E+02    0.67638E-02
 TOTAL         0.13158E+05
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CONNECTED STREAMS.

                 PLATE NO.  1  FROM 24
                 LB MOL/TIME    MOL FRAC
 H2S             0.21813E+01   0.86438E-03
 CO2             0.43463E+01   0.17223E-02
 MEA             0.12735E+03   0.50465E-01
 WATER           0.23897E+04   0.94695E+00
 HYDROGEN        0.42757E-26   0.16944E-29
 NITROGEN        0.29917E-25   0.11855E-28
 METHANE         0.49119E-25   0.19464E-28
 ETHANE          0.22284E-25   0.88305E-29
 PROPANE         0.91632E-26   0.36311E-29
 N-BUTANE        0.60766E-28   0.24080E-31
 I-BUTANE        0.60766E-28   0.24080E-31
 TOTAL           0.25235E+04

 MAKEUP OF AMINE=   0.98816E-01
           WATER=   0.54318E+02

                 PLATE NO.  5  FROM 17
                 LB MOL/TIME    MOL FRAC
 H2S             0.37795E+01   0.14822E-02
 CO2             0.66498E+01   0.26078E-02
 MEA             0.10184E+03   0.39937E-01
 WATER           0.24377E+04   0.95597E+00
 HYDROGEN        0.25686E-17   0.10073E-20
 NITROGEN        0.26894E-19   0.10547E-22
 METHANE         0.28455E-16   0.11159E-19
 ETHANE          0.13168E-16   0.51638E-20
 PROPANE         0.55068E-17   0.21595E-20
 N-BUTANE        0.30226E-19   0.11853E-22
 I-BUTANE        0.30226E-19   0.11853E-22
 TOTAL           0.25500E+04

                 PLATE NO. 12  FROM 10
                 LB MOL/TIME    MOL FRAC
 H2S             0.41782E+02   0.81903E-02
 CO2             0.50933E+02   0.99842E-02
 MEA             0.22910E+03   0.44909E-01
 WATER           0.47782E+04   0.93666E+00
 HYDROGEN        0.46484E-01   0.91121E-05
 NITROGEN        0.34485E+00   0.67600E-04
 METHANE         0.54499E+00   0.10683E-03
 ETHANE          0.24715E+00   0.48449E-04
 PROPANE         0.11429E+00   0.22404E-04
 N-BUTANE        0.47854E-03   0.93807E-07
 I-BUTANE        0.47854E-03   0.93807E-07
 TOTAL           0.51013E+04
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PRODUCTS

                TOP PRODUCT ( 1)            BOTTOM PRODUCT (10)
           LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S       0.11069E+00  0.84298E-05   0.41782E+02  0.81903E-02
 CO2       0.43921E-02  0.33450E-06   0.50933E+02  0.99842E-02
 MEA       0.63161E-01  0.48103E-05   0.22910E+03  0.44909E-01
 WATER     0.53522E+02  0.40762E-02   0.47782E+04  0.93666E+00
 HYDROGEN  0.49999E+03  0.38079E-01   0.46484E-01  0.91121E-05
 NITROGEN  0.50001E+04  0.38080E+00   0.34485E+00  0.67600E-04
 METHANE   0.39998E+04  0.30462E+00   0.54499E+00  0.10683E-03
 ETHANE    0.25000E+04  0.19039E+00   0.24715E+00  0.48449E-04
 PROPANE   0.89995E+03  0.68540E-01   0.11429E+00  0.22404E-04
 N-BUTANE  0.89007E+02  0.67787E-02   0.47854E-03  0.93807E-07
 I-BUTANE  0.89007E+02  0.67787E-02   0.47854E-03  0.93807E-07
 TOTAL     0.13130E+05                0.51013E+04

                TOP PRODUCT (11)            BOTTOM PRODUCT (24)
           LB MOL/TIME   MOL FRAC      LB MOL/TIME   MOL FRAC
 H2S       0.35823E+02  0.43569E+00   0.21807E+01  0.88319E-03
 CO2       0.39946E+02  0.48584E+00   0.43451E+01  0.17598E-02
 MEA       0.45405E-03  0.55223E-05   0.12725E+03  0.51537E-01
 WATER     0.51564E+01  0.62715E-01   0.23353E+04  0.94582E+00
 HYDROGEN  0.46483E-01  0.56535E-03   0.42746E-26  0.17312E-29
 NITROGEN  0.34485E+00  0.41942E-02   0.29909E-25  0.12113E-28
 METHANE   0.54499E+00  0.66284E-02   0.49105E-25  0.19888E-28
 ETHANE    0.24715E+00  0.30060E-02   0.22278E-25  0.90226E-29
 PROPANE   0.11429E+00  0.13901E-02   0.91607E-26  0.37101E-29
 N-BUTANE  0.47853E-03  0.58201E-05   0.60749E-28  0.24604E-31
 I-BUTANE  0.47853E-03  0.58201E-05   0.60749E-28  0.24604E-31
 TOTAL     0.82221E+02                0.24691E+04


LIQUID SIDE STREAMS

                  LIQUID (17)
           LB MOL/TIME    MOL FRAC
 H2S       0.37795E+01   0.14822E-02
 CO2       0.66498E+01   0.26078E-02
 MEA       0.10184E+03   0.39937E-01
 WATER     0.24377E+04   0.95597E+00
 HYDROGEN  0.25686E-17   0.10073E-20
 NITROGEN  0.26894E-19   0.10547E-22
 METHANE   0.28455E-16   0.11159E-19
 ETHANE    0.13168E-16   0.51638E-20
 PROPANE   0.55068E-17   0.21595E-20
 N-BUTANE  0.30226E-19   0.11853E-22
 I-BUTANE  0.30226E-19   0.11853E-22
 TOTAL     0.25500E+04
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